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DISSOCIATION RATE OF BROMINE DIATOMICS IN AN ARGON HEAT BATH

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16. Abstract

The evolution of a collection of 300 K bromine diatomics embedded in a heat bath of argon atoms at 1800 K was studied by computer, and a dissociation-rate constant for the reaction $Br_2 + Ar \rightarrow Br + Br + Ar$ was determined. Previously published probability distributions for energy and angular momentum transfers in classical three-dimensional Br_2-Ar collisions were used in conjunction with a newly developed Monte-Carlo scheme for this purpose. Results are compared with experimental shock-tube data and the predictions of several other theoretical models. A departure from equilibrium is obtained which is significantly greater than that predicted by any of these other theories.

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SUMMARY

The evolution of a collection of 300 K bromine diatomics embedded in a heat bath of argon atoms at 1800 K was studied by computer. Previously published probability distributions for energy and angular momentum transfers in classical three-dimensional collisions were used in conjunction with a newly developed Monte-Carlo scheme to describe the evolution of internal energy and to compute the dissociation rate for the diatomic species. Results are compared with experimental shock-tube data of Warshay and with predictions of other theoretical models. Vibration-rotation coupling in the diatomic is found to play an important role in energy transfer; and a considerable departure from equilibrium is predicted for the internal energy, which greatly exceeds that obtained with any of the other theoretical models. Details of the calculation technique, which can be used to study other molecular systems of comparable complexity, are also presented and discussed.

INTRODUCTION

Experimental shock-tube measurements of dissociation rates for diatomic molecules performed over the last several years have led to extensive discussions regarding the validity of many theoretical models for chemical rate processes (ref. 1). This report attempts to use the basic principles of classical mechanics to provide an understanding of dissociation mechanisms from a microscopic point of view. It also attempts to provide a method for calculating reaction rates for diatomic systems where direct measurements are difficult. To accomplish this, a three-dimensional molecular collision model was constructed for the Br_2-Ar system (refs. 2 and 3), for which extensive measurements are available. This model, which could be used for any atom-diatomic system with an appropriate change in interaction parameters and reduced masses, is believed to be realistic in that most of the more common simplifying assumptions used in various molecular collision theories are absent. Among such simplifications are

assumptions such as collinear collisions, planar motion, impulsive energy transfer ("sudden approximation" and/or hard-sphere models), adiabatic collisions with net energy transfer only upon dissociation, and the neglect of interactions between energy modes (such as vibration-rotation coupling in the diatomic). The present calculations assume that the dissociation mechanism for the diatomic is one involving only collisional energy transfer between atoms of a heat bath and molecules in the electronic ground state and that an atom-molecule encounter can be adequately treated from the point of view of classical mechanics.

Preliminary results with the present collision model (refs. 2 and 3) indicate that vibration-rotation coupling in the Br_2 molecule is very extensive in a heat bath of Ar atoms at 1800 K and that this coupling is likely to play a significant role in the mechanism of atom-diatom energy transfer. Previously published Monte-Carlo calculations of probability distributions for energy and angular momentum changes per collision (refs. 2 and 3) are updated in this report (appendix D) and are used in a new calculation scheme to extract a dissociation rate for the reaction $Br_2 + Ar \rightarrow Br + Br + Ar$. This is compared with experimental measurements performed at a Br_2:Ar concentration ratio of 1:99, where temperature and pressure changes caused by the reaction are insignificant.

In the laboratory the concentration of Br_2 molecules is monitored as a function of time, and a plot of $\ln[Br_2]$ versus time yields a curve whose slope gives the dissociation-rate constant. On the computer a rate constant is determined by a sequence of steps that starts by randomly selecting molecules with internal energies corresponding to a heat bath at the preshocked temperature (300 K) and embedding these in a heat bath at the shocked-gas temperature (1800 K). First, one molecule is selected, embedded in the 1800 K heat bath, and allowed to undergo successive collisions until it dissociates. Then a second molecule is selected and allowed to undergo the same process, and so on for a statistical sample of molecules. The fraction of the sample of molecules remaining undissociated after a given number of collisions is then plotted against the number of collisions. The slope of such a plot yields a dissociation-rate constant in terms of the number of collisions required to dissociate the molecules. This rate constant is finally multiplied by the mean free time for atom-molecule encounters. The result is a rate constant in terms of time, which can be directly compared with an experimental measurement.

The calculation scheme and the use of single-collision probability distributions are discussed in detail and compared to other possible Monte-Carlo procedures for extracting a rate which would ordinarily be prohibitive from the standpoint of computer time. Various features of the evolution of a system of Br_2 diatomics in a heat bath of Ar atoms are also considered.

BASIC CONCEPTS

Symbols used in this report are listed in appendix A, together with numerical values of pertinent physical constants. Unless otherwise stated, all data are presented in scaled SI units defined therein.

Review of Collision Model

The collision model has been presented previously (refs. 2 and 3) but is reviewed here for the reader's convenience. The coordinate system is shown in figure 1, where

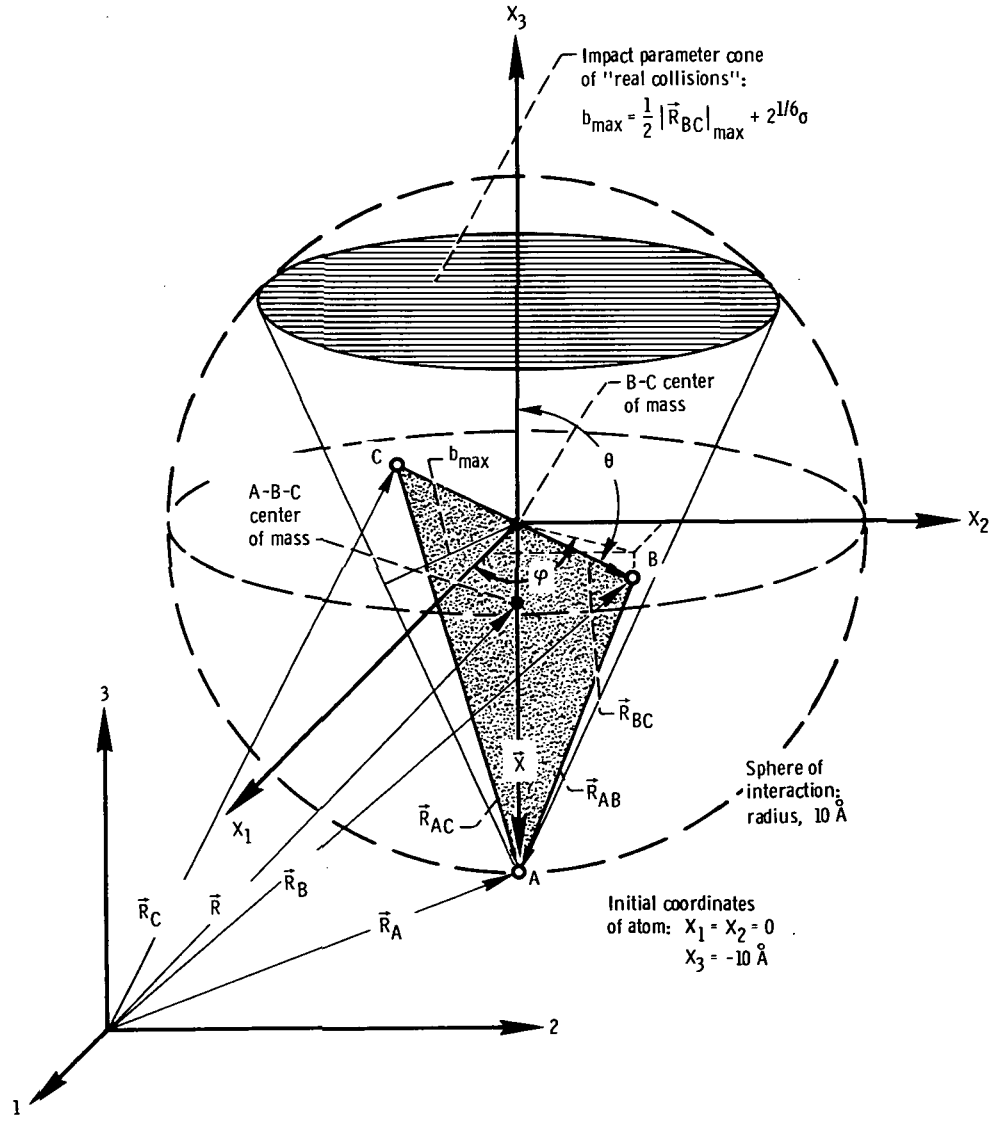


Figure 1. - Coordinate system for three-body problem.

B-C represents the diatomic molecule and A the atom. The total Hamiltonian governing the three-body motion is

$$H = H_{CM} + H_{ABC}$$

where

$$H_{CM} = \frac{1}{2} m_{ABC} |\dot{\vec{R}}|^2 \tag{1}$$

$$H_{ABC} = \frac{1}{2} \mu_{BC} |\dot{\vec{R}}_{BC}|^2 + \frac{1}{2} \mu_{A,BC} |\dot{\vec{X}}|^2 + V_1\left(|\vec{R}_{BC}|\right) + V_2\left(|\vec{R}_{AB}|\right) + V_2\left(|\vec{R}_{AC}|\right) \tag{2}$$

with reduced masses given by $\mu_{BC} = m_B m_C / m_{BC}$ and $\mu_{A,BC} = m_A m_{BC} / m_{ABC}$. The H_{CM} is the kinetic energy of the A-B-C center of mass and is a constant of the motion. The vector $\vec{R}_{BC}$ locates particle B relative to particle C, while the vector $\vec{X}$ locates the atom relative to the center of mass of B-C.

Interactions are taken to act along lines joining the particles and are given by

$$V_1\left(|\vec{R}_{BC}|\right) = \sum_{j=1}^{3} D_j \left\{1 - \exp\left[-\alpha_j\left(|\vec{R}_{BC}| - |\vec{R}_{BC}(e)|\right)\right]\right\}^2 \tag{3}$$

$$V_2\left(|\vec{R}_{AB}|\right) = 4\epsilon\left[\left(\frac{\sigma}{|\vec{R}_{AB}|}\right)^{12} - \left(\frac{\sigma}{|\vec{R}_{AB}|}\right)^{6}\right] \tag{4}$$

$$V_2\left(|\vec{R}_{AC}|\right) = 4\epsilon\left[\left(\frac{\sigma}{|\vec{R}_{AC}|}\right)^{12} - \left(\frac{\sigma}{|\vec{R}_{AC}|}\right)^{6}\right] \tag{5}$$

Equation (3) is a potential in the form of a sum of Morse functions, which was fitted to an RKR potential for the Br-Br ground-state interaction (ref. 3, appendix B). This amounts to using spectroscopic information for the potential. Equations (4) and (5) are Lennard-Jones (6-12) potentials representing the atom-molecule interaction. This pairwise additivity of forces acting along lines joining particles A, B, and C has previously been shown to be adequate for present purposes (ref. 3, p. 12).

Hamilton's equations for the relative A-B-C motion are given by

$$\left.\begin{aligned}
\dot{\vec{R}}_{BC} &= \frac{\partial H}{\partial \vec{P}_{BC}} = \frac{\vec{P}_{BC}}{\mu_{BC}} \\
-\dot{\vec{P}}_{BC} &= \frac{\partial H}{\partial \vec{R}_{BC}} = \frac{\vec{i}_{BC}\partial V_1\left(|\vec{R}_{BC}|\right)}{\partial |\vec{R}_{BC}|} - \frac{(m_C/m_{BC})\vec{i}_{AB}\partial V_2\left(|\vec{R}_{AB}|\right)}{\partial |\vec{R}_{AB}|} \\
&\qquad + \frac{(m_B/m_{BC})\vec{i}_{AC}\partial V_2\left(|\vec{R}_{AC}|\right)}{\partial |\vec{R}_{AC}|} \\
\dot{\vec{X}} &= \frac{\partial H}{\partial \vec{P}} = \frac{\vec{P}}{\mu_{A,BC}} \\
-\dot{\vec{P}} &= \frac{\partial H}{\partial \vec{X}} = \frac{\vec{i}_{AB}\partial V_2\left(|\vec{R}_{AB}|\right)}{\partial |\vec{R}_{AB}|} + \frac{\vec{i}_{AC}\partial V_2\left(|\vec{R}_{AC}|\right)}{\partial |\vec{R}_{AC}|}
\end{aligned}\right\} \qquad (6)$$

where $\vec{P}_{BC}$ and $\vec{P}$ are momenta conjugate to $\vec{R}_{BC}$ and $\vec{X}$, respectively, and $\vec{i}_{jk} = \vec{R}_{jk}/|\vec{R}_{jk}|$ are unit vectors. With the coupling constant ϵ set equal to zero, the equations of motion describe a free atom and free vibrating rotator with any vibration-rotation interaction that may be present. The source of such interaction, which has previously been shown to be significant for Br_2 (refs. 2 and 3), is seen when the internal energy H_{BC} is written as a sum of vibrational and rotational components:

$$H_{BC} = H_v + H_r$$

where

$$\left.\begin{aligned}
H_v &= \left(2\,\mu_{BC}\right)^{-1}\left(\vec{i}_{BC}\cdot\vec{P}_{BC}\right)^2 + V_i\left(|\vec{R}_{BC}|\right) \\
H_r &= \frac{|\vec{M}_{BC}|^2}{2\,\mu_{BC}|\vec{R}_{BC}|^2}
\end{aligned}\right\} \qquad (7)$$

with $\vec{M}_{BC} = \vec{R}_{BC} \times \vec{P}_{BC}$. Here H_v is the energy associated with motion along the bond, and H_r is the energy associated with motion perpendicular to the bond. As a free molecule vibrates, $|\vec{R}_{BC}|$ changes. But for a free molecule, H_{BC} and $|\vec{M}_{BC}|^2$ are constants of the motion, so that any increase in $|\vec{R}_{BC}|$ must result in a decrease in H_r and an increase in H_v. In atom-molecule trajectories, where the molecule is no longer free, H_v-H_r coupling can play a significant role in energy transfer. An example of the excitation of such coupling in an atom-molecule trajectory with H_r initially set equal to zero is shown in figure 2, where H_A is the relative kinetic energy of the atom

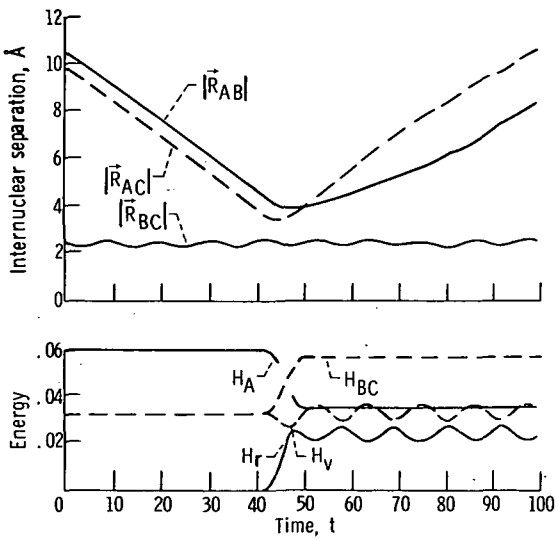


Figure 2. - Atom-molecule trajectory.

(see also ref. 2, fig. 3; and ref. 3, figs. 4 and 5). In this trajectory a large portion of the relative translational energy was converted into rotational energy, after which the coupling between H_v and H_r is a significant factor in the partitioning of internal energy modes.

This partitioning of the energy H_{BC} into H_v and H_r contains all interaction between energy modes implicitly, where H_{BC} reduces to a pure vibrational energy as $|\vec{M}_{BC}|^2 \to 0$ and to a pure rotational energy as $H_v \to 0$. An illustration of what this partitioning implies for a concept of "vibrational energy levels" is shown in figure 3, where H_v for a constant value of H_{BC} is sketched at various values of $|\vec{M}_{BC}|^2$. The potential curve V_1 for the diatomic is the same regardless of the existence of rotation, whereas vibrational energy levels are not horizontal lines intersecting the curve V_1 at classical turning points corresponding to a single value of H_v (except at $|\vec{M}_{BC}|^2 = 0$). It has been previously found (refs. 2 and 3) that for Br_2 in a heat bath

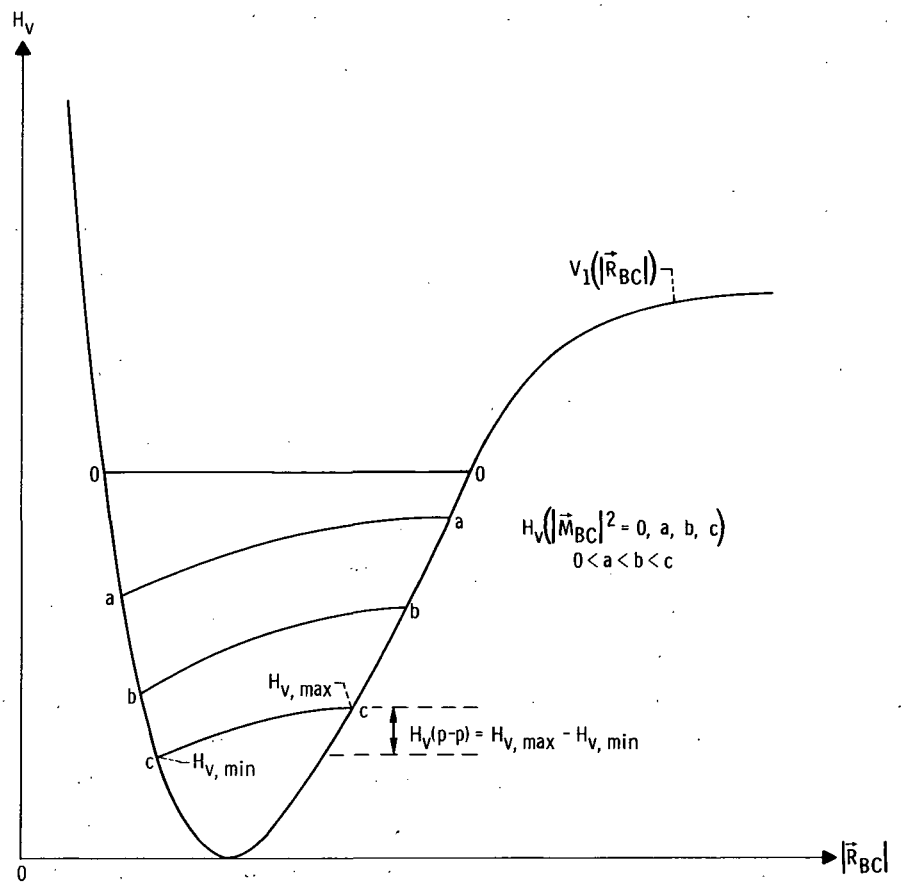


Figure 3. - Classical visualization of "vibrational energy levels" in vibration-rotation coupling for a free diatomic B-C, where a fixed internal energy H_{BC} is partitioned into a sum of instantaneous vibrational and rotational parts $H_{BC} = H_v + H_r$.

of Ar atoms at 1800 K the amplitude of coupling for a single "level" can commonly exceed the spacing of successive quantum vibrational levels based on RKR calculations (zero angular momentum). The amplitude of coupling $H_v(p\text{-}p) = H_{v,max} - H_{v,min}$ is shown in figure 3; and a single "level" refers to classical motion at constant H_{BC} and a given value of $|\vec{M}_{BC}|^2$.

For given initial conditions the equations of motion (in Cartesian coordinates) were integrated on an IBM 7094 computer. Usually, we employed a variable step-size routine which uses the principle of conservation of the energy H_{ABC} to choose an optimum step-size at each time-step interval in the numerical integration (refs. 2 and 3). Energy conservation for a trajectory was required to hold to within a predetermined maximum tolerance of 0.1 percent. This tolerance, in turn, determined uncertainty levels for a trajectory of 0.0001 u for energy and 0.001 $m^2\text{Å}^2v^2$ for angular momentum squared. For some initial conditions, trajectories could not be calculated with sufficient accuracy by using the variable-step-size routine, whereupon a small

fixed time-step of 0.25 t was used. In such cases, however, it was convenient to use the same uncertainty levels for statistical tabulations of energy and angular momentum changes. The correctness of the two integration methods was verified by checking time-reversal invariance.

In present calculations, probability distributions were determined for a molecule, with a given internal energy and angular momentum squared, undergoing changes $\left(\Delta H_{BC}, \Delta|\vec{M}_{BC}|^2\right)$ in a single collision with an atom chosen at random from a heat bath at $T_2 = 1800$ K. These were, in turn, used to calculate a dissociation rate by a scheme that will be described in the subsequent section Calculation of a Dissociation Rate Constant. To determine probability distributions for $\left(\Delta H_{BC}, \Delta|\vec{M}_{BC}|^2\right)$ changes, a sphere of interaction is first circumscribed about the center of mass of the molecule (see fig. 1) with a radius such that for larger distances of the atom from the B-C center of mass, atom trajectories are straight lines to within limits of error in the integration. This radius was determined empirically to be 10 Å (refs. 2 and 3). A collision is then, by definition, a trajectory for the relative A-B-C motion which is determined while the atom is within this radius of interaction. For each trajectory the molecular orientation and angular momentum vector for a molecule with specified initial values of H_{BC} and $|\vec{M}_{BC}|^2$ were randomly distributed over a sphere. An atom was then placed initially on the sphere of interaction. The magnitude of its relative momentum $|\vec{P}|$ was chosen from a Maxwell-Boltzmann flux distribution corresponding to the heat-bath temperature, while the orientation of this momentum was randomly distributed over a half sphere. The trajectory was then followed from $|\vec{X}| = 10$ Å with $|\dot{\vec{X}}| < 0$ to $|\vec{X}| = 10$ Å with $|\dot{\vec{X}}| > 0$, after which the changes $\left(\Delta H_{BC}, \Delta|\vec{M}_{BC}|^2\right)$ for that trajectory were noted. If this is repeated many times for a molecule with specified initial values of H_{BC} and $|\vec{M}_{BC}|^2$, a statistical distribution of trajectories spanning all possible collision orientations and impact parameters (from 0 to 10 Å) is obtained. From these trajectories, probability distributions for ΔH_{BC} and $\Delta|\vec{M}_{BC}|^2$ per collision corresponding to the given initial H_{BC} and $|\vec{M}_{BC}|^2$ can be constructed. Formulas for randomly orienting a molecule and randomly selecting an atom from a heat bath are derived in references 2 and 3 and are summarized in appendix C.

Two types of trajectories were calculated for the present work: those where the initial internal energy $H_{BC}(i)$ was small enough so that $H_{v,max}$ was much less than the dissociation energy D_e, and those where $H_{BC}(i)$ was large enough to bring $H_{v,max}$ very close to D_e (where D_e is the value of V_1 at $|\vec{R}_{BC}| \to \infty$). For trajectories of the former type (to $H_{BC}(i) = 0.9\, D_e$), integration of the equations of motion was actually carried out only if the impact parameter b was less than or equal to a maximum impact parameter defined by $b_{max} = \frac{1}{2}|\vec{R}_{BC}|_{max} + 2^{1/6}\sigma$, where $|\vec{R}_{BC}|_{max}$ is the outer classical turning point in the vibrational motion that would be reached if H_v at

$|\vec{R}_{BC}| = |\vec{R}_{BC}(e)|$ remained unchanged throughout the vibrational period. (A trajectory was always started with $|\vec{R}_{BC}| = |\vec{R}_{BC}(e)|$. See appendix C for details.) Trajectories within the cone defined by b_{max} (see fig. 1) were called real collisions (RCOL), and those outside this cone were called null collisions (NCOL). These latter cases, although not calculated, were nevertheless counted as events for the determination of the distributions for energy and angular momentum changes in a collision. Trajectories with $b > b_{max}$ were found, by trial, not to contribute significantly to overall energy and angular momentum transfers. Hence, they were assigned changes $\Delta H_{BC} = 0$, $\Delta|\vec{M}_{BC}|^2 = 0$.

Calculations where $H_{BC}(i)$ brings $H_{v,max}$ close to D_e present a special problem in that the molecule can dissociate during a trajectory. Dissociation was defined as the instantaneous condition $H_{v,max} \geq 0.9999\ D_e$. This definition corresponds to a finite internuclear separation $|\vec{R}_{BC}| \geq 7.250$ Å and is necessitated in a practical calculation because $H_v \geq D_e$ with the corresponding condition $|\vec{R}_{BC}| \to \infty$ cannot be handled by the computer. With this definition the maximum internal energy $H_{BC,max}$ that a free molecule can have without dissociating was determined to be

$$\frac{H_{BC,max}}{D_e} < 0.9999 + y|\vec{M}_{BC}|^2 \tag{8}$$

where energies and angular momentum squared are expressed in scaled units and $y = 0.0100 \pm 0.0001\ \left(m^2 Å^2 v^2\right)^{-1}$ (ref. 3, eq. (10)). This energy was determined empirically from a series of dummy trajectories ($\epsilon = 0$) as the internal energy above which $|\vec{R}_{BC}|$ would reach 7.250 Å within one vibrational period after the start of a trajectory calculation and continue increasing indefinitely. This empirical value of y is 2.2 times greater than the value of $\left(2\,\mu_{BC}|\vec{R}_{BC}|^2 D_e\right)^{-1}$ that would be obtained from the relation $H_{BC,max} = 0.9999\ D_e + H_r$ (eq. (7)). This empirical value may be the result either of vibration-rotation coupling or perhaps of small errors due to a finite step-size when integrating the equations of motion. At any rate, we felt that for calculation purposes it was better to use the empirically determined value of y in defining the conditions that constitute a dissociation. A constant step-size was used to integrate the equations of motion when the molecule was near dissociation (and also for the condition $H_{BC}(i) = 0$), while a variable step-size was used for all other cases.

To determine probability distributions for $\left(\Delta H_{BC}, \Delta|\vec{M}_{BC}|^2\right)$ with $H_{BC}(i)$ near $H_{BC,max}$, all trajectories were calculated ($b_{max} = 10$ Å) because it was found that large impact parameters could significantly influence the fraction of dissociation events. In reference 3, preliminary calculations of this type were reported, where b_{max} was chosen to be 7.966 Å. This choice was thought to be adequate at the time, based on cal-

culations for small angular momenta. However, extensive subsequent calculations have shown an unexpectedly large sensitivity of the fraction of dissociations to angular momentum and also that the trajectory calculations should be cut off at $|\vec{X}| \geq 10$ Å, and not at $|\vec{X}| \geq 10$ Å or $H_v \geq 0.9999\ D_e$ - whichever occurs first - as was done in reference 3. Consequently, data in this report pertinent to dissociation should be considered to supersede corresponding data in reference 3 except that for vibration-rotation coupling (ref. 3, fig. 3), which remains unchanged.

Calculation of a Dissociation-Rate Constant

In the laboratory the rate of the reaction $Br_2 + Ar \rightarrow Br + Br + Ar$ is measured by monitoring either the rate of disappearance of Br_2 molecules or the rate of appearance of Br atoms. The differential equation governing this reaction is

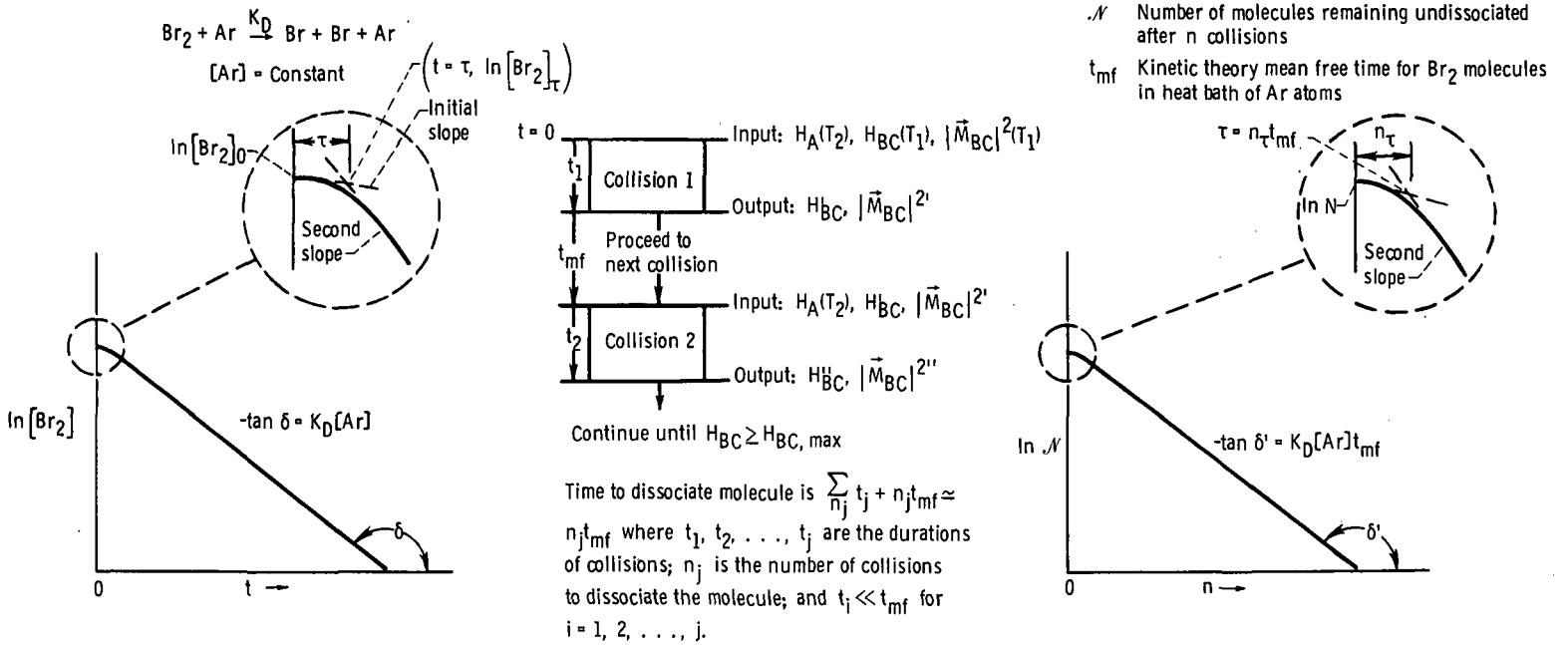
$$\frac{d[Br_2]}{dt} = -K_D[Br_2][Ar] \tag{9}$$

The solution to this equation for times greater than an induction period τ is

$$[Br_2] = \left[Br_2\right]_\tau \exp\left(-\left\{K_D[Ar](t - \tau)\right\}\right) \tag{10}$$

so that a plot of $\ln\left([Br_2]/\left[Br_2\right]_0\right)$ against t is a straight line for $t > \tau$ whose slope is $-\tan\delta = K_D[Ar]$, figure 4(a). (The subscripts 0 and τ indicate the concentration at $t = 0$ and $t = \tau$, respectively.) In shock-tube experiments, rates are extracted from second slopes in such plots (ref. 4, fig. 3) - where the induction period is usually of too short a duration to be measured, and where the slope labeled "second slope" in figure 4 is often referred to as an "initial slope."

On the computer a shock-tube experiment is simulated in the following manner: It is assumed that when the gas is shocked, the translational temperatures of all species in the gas mixture instantaneously jump from the preshocked temperature T_1 to the shocked-gas (heat-bath) temperature T_2, while at the same instant (defined as time zero) internal degrees of freedom (vibration and rotation of the molecule) still correspond to conditions at T_1. The latter then undergo a "relaxation" for $t > 0$, where as a result of energy transfer from translational to vibrational and rotational modes of motion, the molecules gain internal energy at the expense of the relative translational energy of the heat bath. In this process the molecules acquire sufficient internal energy



(a) Plot of laboratory data, with induction period τ exaggerated for illustration.

(b) Schematic of a computer calculation for a single molecule with initial internal energy and angular momentum corresponding to preshock temperature T_1, undergoing successive collisions to dissociation with atoms selected at random from a heat bath at shocked-gas temperature T_2.

(c) Rate calculation by computer using collision model with Monte-Carlo sampling.

Figure 4. - Comparison of a laboratory measurement of a rate constant K_D with a Monte-Carlo computer calculation using collision model.

to dissociate after a number of collisions n_j (fig. 4(b)). The time required to dissociate a given molecule is equal to the sum of the durations of all the collisions $(t_1 + t_2 + \ldots)$ and the product of the total number of collisions by the mean free time $(n_j t_{mf})$. This assumes that the number of collisions is great enough so that the intervals between collisions can be adequately represented, on the average, by a mean free time. Durations of collisions ($\sim 10^2$ scaled t units) are small compared to the mean free time in present calculations. Thus, to a good approximation the time to dissociation is simply the product of the number of collisions by the mean free time. If a collection of such molecules, with internal conditions initially selected at random from a Maxwell-Boltzmann distribution at T_1 (appendix C), are now allowed to undergo successive collisions with atoms randomly selected from a heat bath at T_2 (one molecule at a time), the result will yield the desired rate constant K_D as shown in figure 4(c).

The conversion of the number of collisions needed for dissociation into time requires a knowledge of the mean free time. This is obtained from the kinetic theory frequency with which a single bromine molecule is likely to encounter an argon atom (ref. 5, p. 154):

$$\bar{Z}_{Br_2,Ar} = \frac{1}{t_{mf}} = N_{Ar}\sigma^2_{Br_2,Ar}\left(\frac{8\pi k T_2}{\mu_{A,BC}}\right)^{1/2} \tag{11}$$

where N_{Ar} is the number of argon atoms per cubic centimeter and $\sigma_{Br_2,Ar}$, as used in kinetic theory, would be the separation of centers on impact if Br_2 and Ar were hard spheres. This formula will be valid as long as t_{mf} is much greater than any single duration of collision. In the present collision model, the atom and molecule are, of course, not hard spheres; and they interact over a considerable range of distance. Probability distributions for $\left(\Delta H_{BC}, \Delta|\vec{M}_{BC}|^2\right)$ as determined from trajectory calculations represent the probable outcome of an event where an atom encounters a molecule at an impact parameter of 10 Å or less. The problem is to interpret the "or less" part of this statement in terms of time. A value of $\sigma_{Br_2,Ar} = 10$ Å would only yield a frequency with which an atom is likely to graze the periphery of the 10-Å sphere of interaction but would not represent a frequency with which an atom is likely to have a closer encounter with the molecule. Thus, a rate constant based on $t_{mf}(10\text{ Å})$ would be unreasonably high; so that to convert a collision number for the present model into time, a value of $\sigma_{Br_2,Ar}$ is needed which is intermediate between the minimum of $b = 0$ and the maximum of $b = 10$ Å. For present purposes we will take $\sigma_{Br_2,Ar} = 3.589$ Å, which is the "effective size" of the molecule estimated from viscosity data (private communication with Roger A. Svehla, NASA Lewis Research Center). But we include

calculations for $\sigma_{Br_2,Ar} = 10$ Å in tabulations of results for comparison.

When equation (11) is used, the slope of the Monte-Carlo plot (fig. 4(c)) becomes

$$-\tan\delta' = K_D[Ar]t_{mf} = K_D\left\{\frac{[Ar]}{N_{Ar}}\right\}\left(\frac{1}{\sigma^2_{Br_2,Ar}}\right)\left(\frac{\mu_{A,BC}}{8\pi kT_2}\right)^{1/2}$$

where the dimensions of the quantities involved are K_D in $cm^3/(mole)(sec)$, $[Ar]$ in $moles/cm^3$, N_{Ar} in $molecules/cm^3$, σ in cm, $\mu_{A,BC}$ in g/molecule, k in erg/(K)(molecule), and T in kelvin, with $[Ar]/N_{Ar} = (1/6.02217\times10^{23})(moles/molecule)$. Thus,

$$-\tan\delta' = K_D\left[1/(6.02217\times10^{23})\right]\left(1/\sigma^2_{Br_2,Ar}\right)\left(\mu_{A,BC}/8\pi kT_2\right)^{1/2} \qquad (12)$$

$$\xrightarrow{T_2 = 1800\ K} \begin{cases} (4.840\times10^{-16})K_D & \text{for } \sigma_{Br_2,Ar} = 10\ Å \\ (3.758\times10^{-15})K_D & \text{for } \sigma_{Br_2,Ar} = 3.589\ Å \end{cases}$$

where $-\tan\delta'$ has units of $collisions^{-1}$.

In addition to the problem of deciding what is a reasonable value for $\sigma_{Br_2,Ar}$, there is a problem associated with the size chosen for the sphere of interaction (10 Å in present calculations). As previously noted, a collision is counted as any event where an atom enters the sphere of interaction. Hence, the apparent number of collisions needed to dissociate a molecule is given by $\sum$(NCOL + RCOL), which would change if the radius of the sphere of interaction were changed. Likewise, a change in the radius of the sphere of interaction will also change the slope of a rate plot. However, from a knowledge of the distribution of impact parameters, we can determine the effect on a collision number resulting from a change in the radius of the sphere of interaction. Impact parameters are distributed so that the fraction of events from $(b/\rho) = 0$ to $(b/\rho) = z$ is $2\int_0^z (b/\rho)d(b/\rho) = \left[(b/\rho)^2\right]_0^z$, where ρ is the maximum impact parameter equal to the radius of the sphere of interaction (ref. 6, p. 4535). Thus, if $(b/\rho) = 1/\sqrt{2}$, $(b/\rho)^2 = 1/2$. For $\rho = 10$ Å, one-half the impact parameters are less than 7.07 Å and one-half are greater. (In actual trajectory calculations, fractions for $(b/\rho)^2$ were within ±0.01 or better of the required ratio for all impact parameter intervals

[0, $(b/\rho) \geq 0.05$].) The effect of doubling ρ would be to increase a total collision count by a factor of 4, while halving ρ would divide the total collision count by 4. In this report, slopes of rate plots represent total collision counts based on the 10-Å sphere of interaction. But these slopes and the accompanying rate constants can easily be revised to correspond to a smaller value of ρ. Such revision would not be meaningful, however, for a value of ρ less than an average b_{max} for the molecule, because this would represent a sphere of interaction too small to include all significant internal energy changes. The minimum value of b_{max} corresponds to $H_{BC} = 0$ and is equal to 5.48 Å. A reasonable average b_{max} for the molecule is about 6 Å, which would cut the total collision count for $\rho = 10$ Å by a factor of 9/25. This would, in turn, increase the slopes of rate plots, and likewise the values of K_D obtained for a given t_{mf}, by a factor of about 2.8. (The problem of properly estimating a total collision count should not be confused with the problem of choosing a value for $\sigma_{Br_2,Ar}$. These are entirely separate matters.)

Limitations of a "Direct" Monte-Carlo Calculation

The most direct approach for calculating a rate would be to follow the scheme in figure 4(b), integrating the equations of motion for each collision for each of the molecules in a Monte-Carlo sample. However, a simple initial estimate shows that the computer time required to do this is likely to be impractical. For a 99-percent argon, 1-percent bromine mixture at a pressure of 0.0343 atmosphere and a temperature T_1 of 300 K, equilibrium shock-tube calculations (ref. 7) indicate that the concentration of argon at a shocked-gas temperature T_2 of 1800 K would be $[Ar] = 5.0143\times10^{-6}$ moles/cm^3, or $N_{Ar} = 3.0197\times10^{18}$ atoms/cm^3. From equation (11) this implies mean free times t_{mf} of 9.65×10^{-11} second for $\sigma_{Br_2,Ar} = 10$ Å and 7.48×10^{-10} second for $\sigma_{Br_2,Ar} = 3.589$ Å. The experimental value for K_D (ref. 1) at 1800 K is

$$K_D = 1.44\times10^{9} \text{ cm}^3/(\text{mole})(\text{sec}) \tag{13}$$

which when combined with t_{mf} yields the number of collisions required to achieve a given degree of dissociation x (with n counted from zero, ignoring the induction period):

$$n(x) = \frac{-\ln(1 - x)}{K_D[Ar]t_{mf}} \tag{14}$$

TABLE I. - ESTIMATE OF NUMBER OF COLLISIONS TO ACHIEVE A GIVEN DEGREE OF DISSOCIATION

Degree of dissociation, x	Number of collisions required to achieve x, n(x)		Number of collisions times kinetic theory mean free time, nt_{mf}, μsec
	For $\sigma_{Br_2, Ar}$ = 10 Å	For $\sigma_{Br_2, Ar}$ = 3.589 Å	
0	0	0	0
.01	1.43×10^4	1.64×10^3	1.4
.05	7.01	9.08	6.8
.10	1.50×10^5	1.94×10^4	14.5
.20	3.21	4.15	31.0
[a].26	4.33	5.60	41.8
.30	5.14	6.65	49.6
.40	7.37	9.50	71.1
.50	9.96	1.28×10^5	96.1

[a]Compare t with ref. 4, fig. 3.

Several values of n(x) are listed in table I. According to equation (14) the half-life of Br_2 should correspond to at least 1.28×10^5 collisions. If it is assumed that about 30 percent of the total collisions are RCOL (refs. 2 and 3), the equations of motion would consequently have to be integrated at least 3.8×10^4 times to dissociate one molecule in a half-life. The amount of computer time required to perform the integration for a single collision is of the order of 10 seconds, so that 3.8×10^5 seconds would be required to compute the dissociation of one of the molecules in question. However, a reasonable estimate for a rate would require a sample size of at least 100, and possibly more than 1000, so that the total computer time would probably be of the order of 10^7 to 10^8 seconds (1/3 to 3 yr) on an IBM 7094. This is completely unreasonable from a cost and time standpoint, and an alternative to a "direct" Monte-Carlo calculation must be sought.

Modified Monte-Carlo Calculation Using Single-Collision Probability Distributions for Energy and Angular Momentum Transfer

As an alternative to integrating the equations of motion for each collision of each molecule whose dissociation is to be simulated, the following scheme was used:

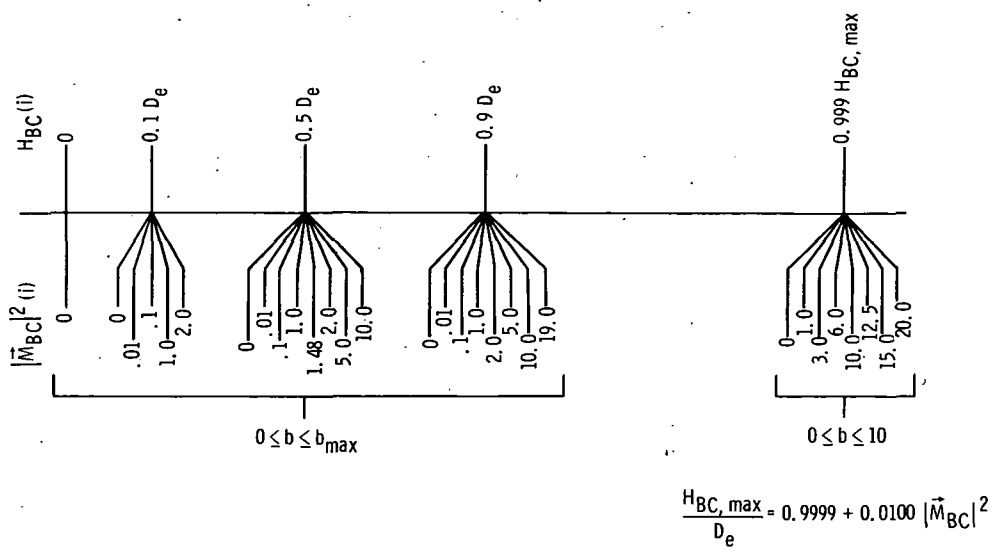


Figure 5. - Initial molecule conditions for which $\left(\Delta H_{BC}, \Delta|\vec{M}_{BC}|^2\right)$ probability distributions were determined and used in Br_2-Ar rate calculation at heat-bath temperature T_2 of 1800 K.

(1) Select a number of initial molecule conditions $\left(H_{BC}(i),\ |\vec{M}_{BC}|^2(i)\right)$ that are representative of undissociated molecules. In this work, 30 sets of initial conditions were chosen, as shown in figure 5.

(2) Simulate a large number of collisions for each set of initial conditions. (The molecule is returned to the initial conditions before each collision.) A simulation corresponds to an integration of the equations of motion for each collision. In this work, 1000 or more trajectories (RCOL) were calculated for each of the 30 sets of initial conditions shown in figure 5.

(3) From the results of 2 construct a two-variable distribution function F_i for all changes $\left(\Delta H_{BC},\ \Delta|\vec{M}_{BC}|^2\right)$ for each set of initial molecule conditions. Then simulation

by integration of the equations of motion can be replaced by randomly selecting a pair $\left(\Delta H_{BC}, \Delta|\vec{M}_{BC}|^2\right)$ from the F_i's. The F_i's are defined in such a way that the set of $\left(\Delta H_{BC}, \Delta|\vec{M}_{BC}|^2\right)$ obtained from many evaluations of F_i has a distribution close to the corresponding set of $\left(\Delta H_{BC}, \Delta|\vec{M}_{BC}|^2\right)$ obtained by integrating the equations of motion.

(4) A random collision of a molecule with arbitrary initial conditions may now be simulated by the interpolation method discussed in appendix B. The results of a collision involving a molecule at arbitrary initial conditions are obtained by interpolation between molecules at the set of 30 fixed initial conditions. Such interpolation will simulate a collision in about 10^{-3} second, instead of the 10 seconds it takes to calculate a trajectory by integrating the equations of motion. Thus, the time necessary for the calculation of a dissociation is down to a reasonable value.

The set $\left(\Delta H_{BC}, \Delta|\vec{M}_{BC}|^2\right)$ obtained for a given set of initial molecule conditions, $\left(H_{BC}(i), |\vec{M}_{BC}|^2(i)\right)$, defines points that lie on a hypersurface in $\left(H_{BC}(i), |\vec{M}_{BC}|^2(i), \Delta H_{BC}, \Delta|\vec{M}_{BC}|^2\right)$ space. A choice of ΔH_{BC} will define a cut on that hypersurface on which lie all the $\Delta|\vec{M}_{BC}|^2$ changes that can accompany the chosen value of ΔH_{BC}. Conversely, a choice of $\Delta|\vec{M}_{BC}|^2$ will define a cut on which lie all ΔH_{BC} changes that can accompany the chosen value of $\Delta|\vec{M}_{BC}|^2$. Changes ΔH_{BC} are not independent of $\Delta|\vec{M}_{BC}|^2$, and conversely (ref. 3, p. 13). That is, for a given probable value of ΔH_{BC}, all $\Delta|\vec{M}_{BC}|^2$ changes are not probable. The problem is to approximate the $\left(\Delta H_{BC}, \Delta|\vec{M}_{BC}|^2\right)$ hypersurface from the finite set of points obtained from trajectory calculations. Since it would not be economically feasible to do sufficient calculations to accurately determine a $\Delta|\vec{M}_{BC}|^2$ cut for each ΔH_{BC} (and conversely), we have made the following approximations: All ΔH_{BC} and $\Delta|\vec{M}_{BC}|^2$ changes were grouped according to orders of magnitude. Then the functions F_i were constructed so that a given order of magnitude for ΔH_{BC} will locate only probable orders of magnitude for $\Delta|\vec{M}_{BC}|^2$. Once an order of magnitude for $\Delta|\vec{M}_{BC}|^2$ has been chosen, we have then assumed that a specific value for $\Delta|\vec{M}_{BC}|^2$ can be chosen from a cumulative distribution for all the $\Delta|\vec{M}_{BC}|^2$ changes in that order of magnitude that occurred in the set $\left(\Delta H_{BC}, \Delta|\vec{M}_{BC}|^2\right)$ - not just those $\Delta|\vec{M}_{BC}|^2$ accompanying the given order of magnitude for ΔH_{BC}. We have constructed the functions F_i such that the selection of a pair $\left(\Delta H_{BC}, \Delta|\vec{M}_{BC}|^2\right)$ is a three-step process involving (1) selection of a specific value for ΔH_{BC} from a cumulative distribution for all ΔH_{BC} changes; (2) use of the order of magnitude of ΔH_{BC} to select an order of magnitude for $\Delta|\vec{M}_{BC}|^2$ from a conditional distribution for orders of magnitude of $\Delta|\vec{M}_{BC}|^2$; (3) selection of a specific value for $\Delta|\vec{M}_{BC}|^2$ from a cumulative distribution for all $\Delta|\vec{M}_{BC}|^2$ changes in the

TABLE II. - EXAMPLE OF FUNCTION F_i IN TABULAR FORM FOR INITIAL CONDITIONS $\left(H_{BC}(i) = 0.1\ D_e,\ |\vec{M}_{BC}|^2(i) = 0.01\right)$ WHERE CHANGES $\left(\Delta H_{BC},\ \Delta|\vec{M}_{BC}|^2\right)$ PER COLLISION ARE MAPPED ONTO THE RANDOM NUMBER INTERVAL $[0, 1]$

SET 3 HBC = (0.1000)DE , MBC2 = 0.01 , T = 1800.

ZH	DELHBC	*	DELHBC RANGE	ZHM	DELMBC2	*	DELMBC2 RANGE	*	DELMBC2 RANGE	ZM	DELMBC2
******	*******	*	*****	******	*****	*	*****		*****	******	*******
0.	-0.0100		-E-01	1.0000	+E-01		-E-02		-E-02	0.	-0.010
0.0003	-0.0090		-E-02	0.0435	-E-02		-E-02		-E-02	0.0635	-0.009
0.0006	-0.0060		-E-02	0.1304	0		-E-02		-E-02	0.1190	-0.008
0.0009	-0.0050		-E-02	0.1739	+E-02		-E-02		-E-02	0.2063	-0.007
0.0013	-0.0040		-E-02	0.5652	+E-01		-E-02		-E-02	0.3254	-0.006
0.0035	-0.0030		-E-02	0.9565	+E 00		-E-02		-E-02	0.3968	-0.005
0.0044	-0.0020		-E-02	1.0000	+E+01		-E-02		-E-02	0.5079	-0.004
0.0076	-0.0010		-E-03	0.6377	-E-02		-E-02		-E-02	0.6270	-0.003
0.0079	-0.0007		-E-03	0.7101	0		-E-02		-E-02	0.7778	-0.002
0.0088	-0.0006		-E-03	0.8116	+E-02		-E-02		-E-02	1.0000	-0.001
0.0104	-0.0005		-E-03	0.9420	+E-01		+E-02		0.		0.001
0.0107	-0.0004		-E-03	0.9710	+E 00		+E-02		0.2150		0.002
0.0113	-0.0003		-E-03	1.0000	+E+01		+E-02		0.3271		0.003
0.0129	-0.0002		0	0.0302	-E-02		+E-02		0.4579		0.004
0.0280	-0.0001		0	0.9656	0		+E-02		0.5607		0.005
0.0281	0.		0	0.9970	+E-02		+E-02		0.6355		0.006
0.7704	0.		0	1.0000	+E+01		+E-02		0.7103		0.007
0.7705	0.0001		+E-03	0.0422	-E-02		+E-02		0.7664		0.008
0.7883	0.0002		+E-03	0.1988	+E-02		+E-02		0.8785		0.009
0.7968	0.0003		+E-03	0.9337	+E-01		+E-02		1.0000		0.010
0.8038	0.0004		+E-03	1.0000	+E 00		+E-01		0.		0.010
0.8091	0.0005		+E-02	0.0054	-E-02		+E-01		0.2718		0.020
0.8121	0.0006		+E-02	0.0081	+E-02		+E-01		0.4308		0.030
0.8167	0.0007		+E-02	0.1297	+E-01		+E-01		0.5897		0.040
0.8198	0.0008		+E-02	0.9892	+E 00		+E-01		0.6769		0.050
0.8214	0.0009		+E-02	1.0000	+E+01		+E-01		0.7436		0.060
0.8227	0.0010		+E-01	0.3125	+E 00		+E-01		0.8103		0.070
0.8491	0.0020		+E-01	1.0000	+E+01		+E-01		0.8821		0.080
0.8683	0.0030						+E-01		0.9744		0.090
0.8825	0.0040						+E-01		1.0000		0.100
0.8964	0.0050						+E 00		0.		0.100
0.9071	0.0060						+E 00		0.2180		0.200
0.9181	0.0070						+E 00		0.3910		0.300
0.9298	0.0080						+E 00		0.5263		0.400
0.9348	0.0090						+E 00		0.6742		0.500
0.9402	0.0100						+E 00		0.7794		0.600
0.9735	0.0200						+E 00		0.8571		0.700
0.9880	0.0300						+E 00		0.8947		0.800
0.9956	0.0400						+E 00		0.9599		0.900
0.9975	0.0500						+E 00		1.0000		1.000
0.9984	0.0600						+E+01		0.		1.000
0.9991	0.0700						+E+01		0.7194		2.000
0.9994	0.0800						+E+01		0.8993		3.000
1.0000	1.0000						+E+01		0.9640		4.000
							+E+01		0.9784		5.000
							+E+01		1.0000		6.000

chosen order of magnitude. The adequacy of these approximations was checked by a procedure outlined in the following section. In this work we have used only the scheme of first selecting ΔH_{BC} and then working to $\Delta|\vec{M}_{BC}|^2$, although it should be possible to reverse the process by constructing alternate functions F_i with the roles of ΔH_{BC} and $\Delta|\vec{M}_{BC}|^2$ interchanged. Although performing calculations by each of these alternate paths would provide the best check of the calculation scheme, time limitations did not permit this to be done.

Construction and Use of Functions F_i

An example of a function F_i in tabular form, which was constructed for initial conditions $\left(H_{BC}(i) = 0.1\ D_e,\ |\vec{M}_{BC}|^2(i) = 0.01\right)$, is given in table II. Similar tabulations for each of the 30 sets of initial conditions (fig. 5) are included in appendix F. (In these tabulations, energy changes are given in scaled energy units, not in fractions of D_e; $\Delta|\vec{M}_{BC}|^2$ is also in scaled units; and exponents on numbers are written so that, for example, the number +0.0040 would correspond to +0.40 E-02.) In table II the first two columns on the left represent a cumulative distribution for ΔH_{BC} changes that occurred in trajectory calculations. These changes can be divided into three kinds: losses where $\Delta H_{BC} \leq -0.0001$ u, nulls where $-0.0001\ u < \Delta H_{BC} < +0.0001$ u, and gains where $\Delta H_{BC} \geq +0.0001$ u (where 0.0001 u is the uncertainty level for energy changes). Losses and gains are decade subdivided in the "DELHBC" column, while nulls are grouped together and assigned a change 0 in this column. The random number interval [0, 1] is then subdivided in the "ZH" column in direct proportion to the number of events in each corresponding DELHBC subinterval that occurred in trajectory calculations. Linear interpolation for ΔH_{BC} is used within each subinterval. The interval $0 \leq ZH \leq 0.0280$ represents the fraction $\sum$(RCOL losses)/$\sum$(RCOL + NCOL) = (0.0280 - 0) = 0.0280; the interval $0.0281 \leq ZH \leq 0.7704$ represents the fraction $\sum$(NCOL + RCOL nulls)/$\sum$(RCOL + NCOL) = (0.7704 - 0.0280) = 0.7424; and the interval $0.7705 \leq ZH \leq 1.0000$ represents the fraction $\sum$(RCOL gains)/$\sum$(RCOL + NCOL) = (1 - 0.7704) = 0.2296 (see also table VI, appendix D). (A jump of 0.0001 in ZH is used at the boundaries between losses-nulls and nulls-gains to avoid the possibility that a given random number might be assigned to two different ΔH_{BC} changes.) This scheme does not distinguish between a RCOL null, for which ΔH_{BC} was within the uncertainty level, and NCOL, for which trajectories were not actually calculated.

The three center columns in table II represent a conditional distribution for the magnitudes of $\Delta|\vec{M}_{BC}|^2$ that accompany a given magnitude of ΔH_{BC}; they account for the fact that ΔH_{BC} and $\Delta|\vec{M}_{BC}|^2$ cannot be treated independently. In the table, each order of magnitude for either ΔH_{BC} or $\Delta|\vec{M}_{BC}|^2$ is labeled a "range." Thus, for

a ΔH_{BC} range of -E-01 only $\Delta|\vec{M}_{BC}|^2$ changes in the range +E-01 occurred in trajectory calculations; for a ΔH_{BC} range of -E-02, $\Delta|\vec{M}_{BC}|^2$ ranges of -E-02, 0, +E-02, +E-01, +E 00, +E+01 occurred, and so on. As with energy, $\Delta|\vec{M}_{BC}|^2$ changes of 0 represent both RCOL for which $-0.001 < \Delta|\vec{M}_{BC}|^2 < +0.001$, where $0.001\ m^2 Å^2 v^2$ is the uncertainty level for angular momentum squared, and NCOL. For each ΔH_{BC} range the random number interval [0, 1] is subdivided in proportion to the number of $\Delta|\vec{M}_{BC}|^2$ changes in a given range that accompanied the stated ΔH_{BC} range in trajectory calculations. In the "ZHM" column a number n_2 corresponds to the upper limit in an interval $n_1 < ZHM \leq n_2$. For example, for the "DELHBC RANGE" of -E-02, the number 0.0435 corresponds to $0 \leq ZHM \leq 0.0435$, the number 0.1304 corresponds to $0.0435 < ZHM \leq 0.1304$, and so on.

The last three columns in table II represent cumulative distributions for each nonzero $\Delta|\vec{M}_{BC}|^2$ range. All $\Delta|\vec{M}_{BC}|^2$ changes of a given range that occurred in trajectory calculations are decade subdivided in the "DELMBC2" column and are proportioned according to the number of occurrences in the "ZM" column. These distributions are used to interpolate for $\Delta|\vec{M}_{BC}|^2$ within a given range, with linear interpolation being used between "DELMBC2" subintervals.

To simulate a collision using the F_i, three random numbers ZH, ZHM, and ZM are chosen. The ZH assigns a definite value for a ΔH_{BC} change and also defines a ΔH_{BC} range. The ZHM then assigns a $\Delta|\vec{M}_{BC}|^2$ range for the collision. If the $\Delta|\vec{M}_{BC}|^2$ range assigned is 0, then $\Delta|\vec{M}_{BC}|^2 = 0$ is assigned for an angular momentum change, and the simulation is completed. If the $\Delta|\vec{M}_{BC}|^2$ range assigned is other than zero, then the ZM is used to assign a definite $\Delta|\vec{M}_{BC}|^2$ change in the required range.

To test the adequacy of the interpolation scheme and the random number mappings, single collision probability distributions were regenerated by randomly choosing values of ΔH_{BC} and $\Delta|\vec{M}_{BC}|^2$ for successive molecules, each with initial conditions corresponding exactly to one of the distributions in figure 5. The $\left(\Delta H_{BC}, \Delta|\vec{M}_{BC}|^2\right)$ changes for a sample of 1000 such molecules were found to be distributed in the same way as the results for the original trajectory calculations (from which the F_i were derived) to better than 1 percent. (That is, the fraction of total events within the uncertainty level and the fractions of gains or losses of a given magnitude or greater matched corresponding fractions for the original trajectory calculations - as given in appendix D - to better than 0.01 for a given fraction.) This verifies that the use of random number mappings, together with the interpolation scheme, can assign random $\left(\Delta H_{BC}, \Delta|\vec{M}_{BC}|^2\right)$ changes to a molecule, such that after many applications of this procedure the distributions of such changes would not differ substantially from statis-

tical results to be expected if the equations of motion were being integrated for every collision.

RESULTS

Summary of Characteristics of Single-Collision Probability Distributions

Probability distributions for energy and angular momentum changes per collision, as calculated by the present model (appendix D), have previously been compared for consistency with results that would be expected from other physical theories, such as rigid rotator collision models, equilibrium statistical mechanics, and thermodynamics (ref. 3, pp. 17-18). Such comparisons provide an evaluation of the usefulness of calculations based on the probability distributions. For example, it was found that the combination of initial conditions and heat-bath temperature ($T_2 \leq 1800$ K) that would result in a gains-losses balance for $\Delta|\vec{M}_{BC}|^2$ (per collision) in the vibrating-rotator corresponded moderately well to $\langle H_r \rangle = kT_2 = \left\langle |\vec{M}_{BC}|^2 \right\rangle / 2\mu_{BC}|\vec{R}_{BC}|^2$. In this expression, $\langle H_r \rangle$ is the mean internal energy for a rigid rotator ($\frac{1}{2}kT_2$ per degree of freedom) with $|\vec{R}_{BC}|$ taken as the average internuclear separation for the vibrating-rotator under the specified conditions, and $\left\langle |\vec{M}_{BC}|^2 \right\rangle$ is the average angular momentum squared at equilibrium for the rigid rotator (ref. 3, p. 17 and table VIII). In another comparison it was found that a combination of initial conditions and heat-bath temperature, $\left(H_{BC}(i),\ |\vec{M}_{BC}|^2(i),\ T_2\right)$, that would lead to a simultaneous gains-losses balance for both ΔH_{BC} and $\Delta|\vec{M}_{BC}|^2$ (per collision) could be obtained if the internal energy and heat-bath temperature were related by $H_{BC}(i) = (3/2)kT_2$ (ref. 3, pp. 17-18).

These comparisons were carried out only for cases where $H_{BC}(i) \ll H_{BC,max}$, equation (8). At the time reference 3 was written, only preliminary results for the molecule near dissociation were available. Extensive studies in this region have since been completed and are summarized in figure 6. Each point in the plot represents the fraction of events where molecules were dissociated in one trajectory in calculations for probability distributions at $H_{BC}(i) = 0.999\ H_{BC,max}$. This plot shows that the probability of dissociating a molecule - with initial conditions such that the outer classical turning point in the vibrational motion is always within 99.9 percent of the computer definition of dissociation - is a sensitive function of the initial angular momentum of the molecule. Beyond $|\vec{M}_{BC}|^2(i) = 9$, the fraction of dissociations drops off sharply. This value of $|\vec{M}_{BC}|^2(i)$ corresponds approximately to the point where the magnitude of the circular velocity (length of arc per unit time) of the Br particles in the rotating

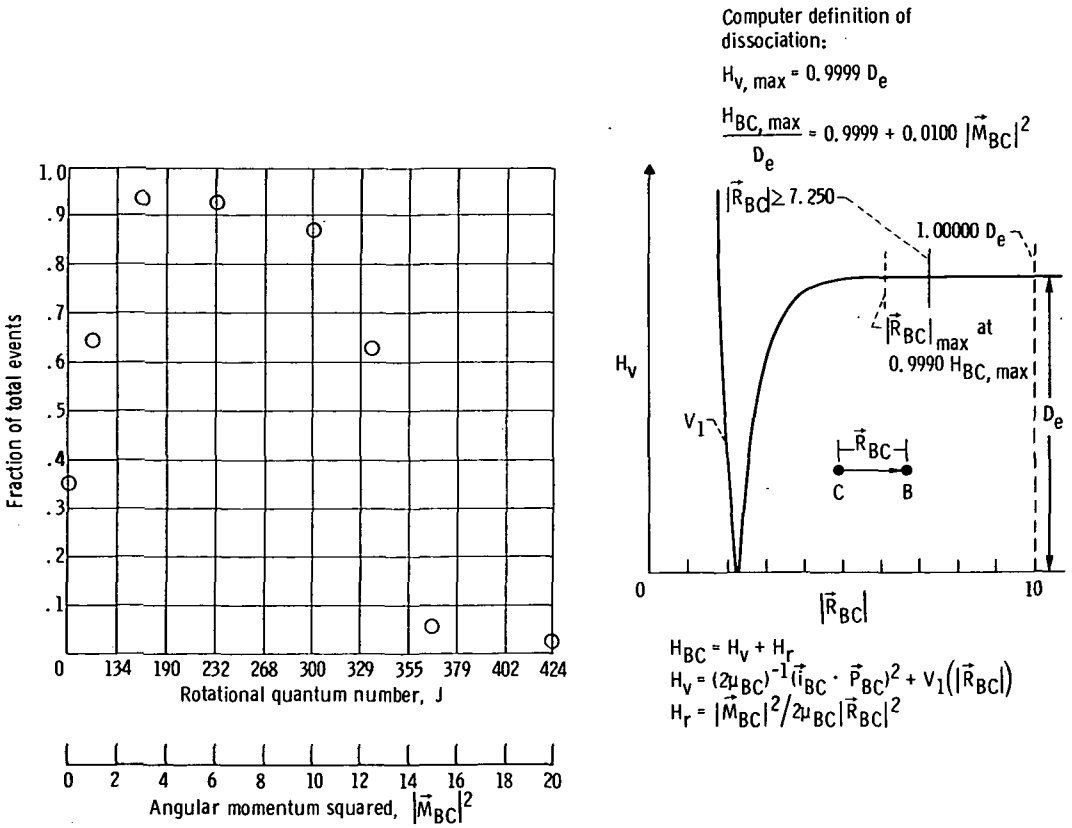


Figure 6. - Probability of dissociating a Br_2 molecule in a single collision with Ar atoms in a heat bath at 1800 K as a function of initial Br_2 angular momentum. The Br_2 molecule has an initial energy H_{BC} such that the outer classical turning point is within 99.9 percent of the computer definition of dissociation. Because of vibration-rotation coupling, the inner classical turning point for the initially free molecule will be less than 99.9 percent of $H_{v,max}$, except for zero angular momentum.

molecule at $|\vec{R}_{BC}| = |\vec{R}_{BC}(e)|$ would equal the magnitude of the peak atom velocity at T_2 = 1800 K (table III). From equation (7), we can deduce that the rate of conversion of H_v into H_r (and conversely) due to H_v-H_r coupling is a maximum whenever $|\dot{\vec{R}}_{BC}|$ is a maximum. Since this maximum in $|\dot{\vec{R}}_{BC}|$ occurs as $|\vec{R}_{BC}|$ passes through $|\vec{R}_{BC}(e)|$, the observed drop in the fraction of dissociations might indicate an increased difficulty in converting translational energy into H_r - and through coupling into H_v - when the circular velocity of the Br particles at $|\vec{R}_{BC}| = |\vec{R}_{BC}(e)|$ exceeds the peak atom velocity.

Reference 3 compares dissociation events accompanied by a gain or loss in $|\vec{M}_{BC}|^2$, based on preliminary calculations near $H_{BC,max}$ (ref. 3, p. 15 and fig. 7). Data for updating this comparison are included in appendix D, table VII, in a column giving the ratio of dissociation events with $|\vec{M}_{BC}|^2$ loss to dissociation events with $|\vec{M}_{BC}|^2$ gain. The basic conclusions remain the same as those given in reference 3.

TABLE III. - COMPARISON OF PEAK ATOM VELOCITY WITH CIRCULAR VELOCITY (LENGTH OF ARC PER UNIT TIME) OF Br PARTICLES IN ROTATING Br_2 MOLECULE

Peak of Maxwell-Boltzmann flux distribution for atom at heat-bath temperature T_2 of 1800 K:

$$kT = 0.0248497\ u = 1/2\ \mu_{A,BC} |\dot{\vec{X}}|^2_{peak}$$

where

$$|\dot{\vec{X}}|_{peak} = 0.0096776\ \text{Å/t unit}$$

Square of angular velocity of Br_2 in plane of rotation (ref. 3, p. 32):

$$|\dot{\Phi}|^2 = \frac{|\vec{M}_{BC}|^2}{\mu^2_{BC} |\vec{R}_{BC}|^4}$$

Length of arc per unit time traversed by Br particles:

$$\frac{\text{Radians/t unit}}{2\pi\ \text{Radians/Circumference}} = |\dot{\Phi}| \cdot \frac{\pi |\vec{R}_{BC}|}{2\pi} = \frac{1}{2} |\dot{\Phi}|\, |\vec{R}_{BC}|$$

$$= \frac{1}{2} \left(\frac{|\vec{M}_{BC}|^2}{\mu^2_{BC} |\vec{R}_{BC}|^2} \right)^{1/2}$$

Angular momentum squared, $\lvert\vec{M}_{BC}\rvert^2$	Length of arc per unit time traversed by Br particles, $1/2\ \lvert\dot{\Phi}\rvert\ \lvert\vec{R}_{BC}\rvert$, at location of particle B relative to particle C, $\lvert\vec{R}_{BC}\rvert$, of -	
	7.250 Å	$\lvert\vec{R}_{BC}(e)\rvert$ = 2.28161 Å
	in Å/t unit	
0	0	0
1	.001040	.003304
2	.001470	.004670
3	.001802	.005730
4	.002079	.006605
6	.002546	.008089
8	.002940	.009340
9	.003118	.009906
10	.003287	.01044
12	.003601	.01144
15	.004030	.01281
20	.004648	.01477

Initial Stage in Evolution of Internal Energy

The initial stage in the evolution of a sample of 10 000 molecules, with internal energies distributed at time zero as a Maxwell-Boltzmann distribution at $T_1 = 300$ K (appendix C) was followed for 200 collisions. The purpose was to determine if an initial Maxwell-Boltzmann distribution of molecules would evolve as a series of such distributions corresponding to higher and higher temperatures. This has been shown to be the case for a gas of harmonic oscillators (refs. 8 and 9) - with no vibration-rotation coupling and where rotational degrees of freedom are in equilibrium with the heat bath. But it has not been previously demonstrated for a system of the complication considered herein (anharmonic vibrating rotators with significant vibration-rotation interaction, and without "rotational equilibrium" throughout the relaxation being assumed).

A detailed computer tabulation of the results is given in appendix E. The average system energy and angular momentum squared for the undissociated portion of the sample are plotted in figure 7. (After 200 collisions, 99.50 percent of the original sample is undissociated.) From this figure it is seen that the system of diatomics undergoes an initial transient characterized by relatively large changes in the average internal energy and angular momentum squared. This transient is nearly complete in 200 col-

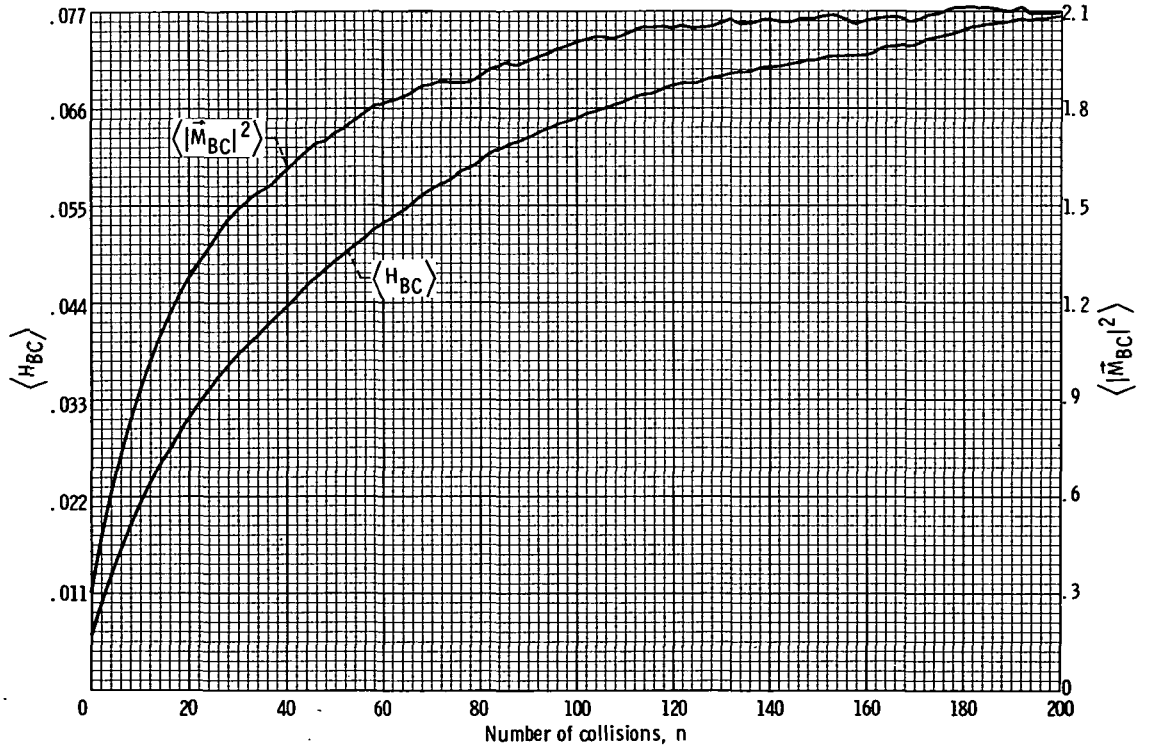


Figure 7. - Initial stage of evolution of 300 K Br_2 diatomics in Ar heat path at 1800 K: average energy and angular momentum squared for sample of 10 000 molecules after n collisions.

lisions, after which the evolution of the system of diatomics is more gradual. The average internal energy changes on about the same time scale as the average angular momentum squared, reflecting the fact that significant internal energy changes are usually accompanied by significant angular momentum changes (ref. 3, pp. 16-17).

From the distribution of energies for the 10 000 molecules after each has experienced n collisions (appendix E), we can decipher how the system of diatomics evolves and, in particular, answer the question of whether a system which starts out with a Maxwell-Boltzmann energy distribution maintains a Maxwell-Boltzmann character as it evolves. We do this by calculating the Maxwell-Boltzmann temperature T_{MB} corresponding to a given fraction of the total sample of molecules that have energies of H_{BC} or greater:

$$f(H_{BC}, T_{MB}) = \left(\frac{2}{\sqrt{\pi}}\right)\left(\frac{1}{kT_{MB}}\right)^{3/2}\int_{H_{BC}}^{\infty}\left(\sqrt{H_{BC}}\right)\exp\left(\frac{-H_{BC}}{kT_{MB}}\right)dH_{BC} \qquad (15)$$

and by ascertaining whether a single value of T_{MB} can be obtained after n collisions regardless of the integral lower limit H_{BC}. For equation (15) $[f]_{H_{BC}=0}^{\infty} = 1$, where the brackets indicate the value of the integral between the specified limits. For molecules initially selected to correspond to $T_1 = T_{MB} = 300$ K at time zero (see appendix C), the required fractions for successive energy ranges at 300 K are $[f]_{0.01}^{\infty} = 0.18475$, $[f]_{0.02}^{\infty} = 0.02171$, and $[f]_{0.03}^{\infty} = 0.00231$, where H_{BC} is expressed in scaled units. By referring to appendix E, we find that, out of a sample of 10 000 randomly selected molecules at $T_1 = 300$ K, 1865 molecules had energies of 0.01 u or greater (301.4 K), 217 had energies of 0.02 u or greater, and 23 had energies of 0.03 u or greater, which corresponds closely to the required starting Maxwell-Boltzmann distribution.

As the sample evolved, fractions of the sample with internal energies at a given level or greater after n collisions were substituted into equation (15), and the result was solved for T_{MB}. If the sample were actually distributed according to a Maxwell-Boltzmann distribution, the same value of T_{MB} after n collisions would be obtained regardless of the energy interval used in solving for T_{MB}. Values of T_{MB} after each collision to $n = 70$ were determined from the tabulations in appendix E for energy intervals corresponding to integral lower limits (eq. (15)) of $H_{BC} = 0.01$, 0.02, 0.03, 0.04, 0.05, 0.06, 0.07, and 0.08. The results are shown in figure 8. (The curve for $H_{BC} = 0.01$ was taken only to $n = 46$ because values of T_{MB} cannot be accurately evaluated for fractions of the total sample greater than 0.9. For such fractions a small portion of the total sample represents a T_{MB} range from $\sim 10^3$ K to infinity.) With a sample size of 10 000 molecules, temperatures can be assigned to fractional energy dis-

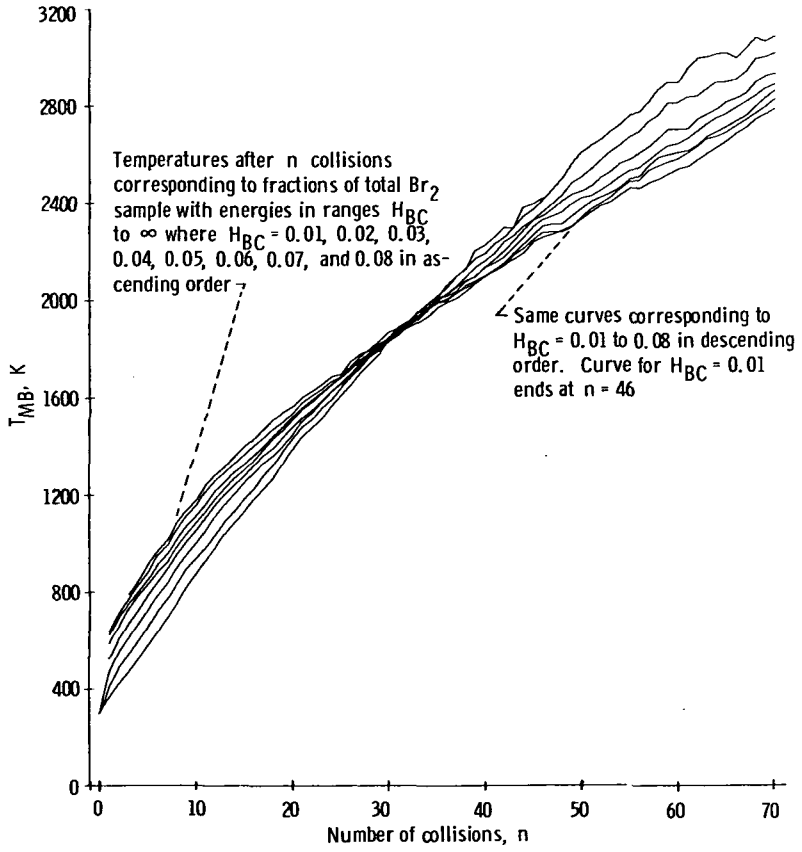


Figure 8. - Maxwell-Boltzmann temperatures T_{MB} corresponding to internal energy distributions of Br_2 after n collisions for 10 000 Br_2 diatomics initially at 300 K embedded in Ar heat bath at 1800 K.

tributions in the ranges $H_{BC} \geq 0.01$ to $H_{BC} \geq 0.08$, usually to within three significant digits below 1000 K and four digits above 1000 K, with a maximum uncertainty of 10 to 20 K attributable to randomness in the Monte-Carlo process. Figure 8 shows that, after the first collision (n = 1), the system that started out as a Maxwell-Boltzmann distribution deviates from such distribution to an extent well beyond the uncertainty in the calculations. As the system relaxes, the T_{MB} curves for the various energy intervals converge and cross. After about 29 collisions the system of diatomics evolves to the point where values of T_{MB} for each curve are about equal to the heat-bath temperature. After 29 collisions and in the vicinity of 29 collisions, the system is instantaneously distributed like - and also evolves very much like - a true Maxwell-Boltzmann distribution. This is shown in figure 9, where the sample distributions after 29 collisions and after 200 collisions are compared with Maxwell-Boltzmann distributions at several temperatures. The point where the Maxwell-Boltzmann character is most closely approximated does not occur exactly at the heat-bath temperature, however, but at a temperature slightly higher. The present system of diatomics appears to "overshoot" the heat-

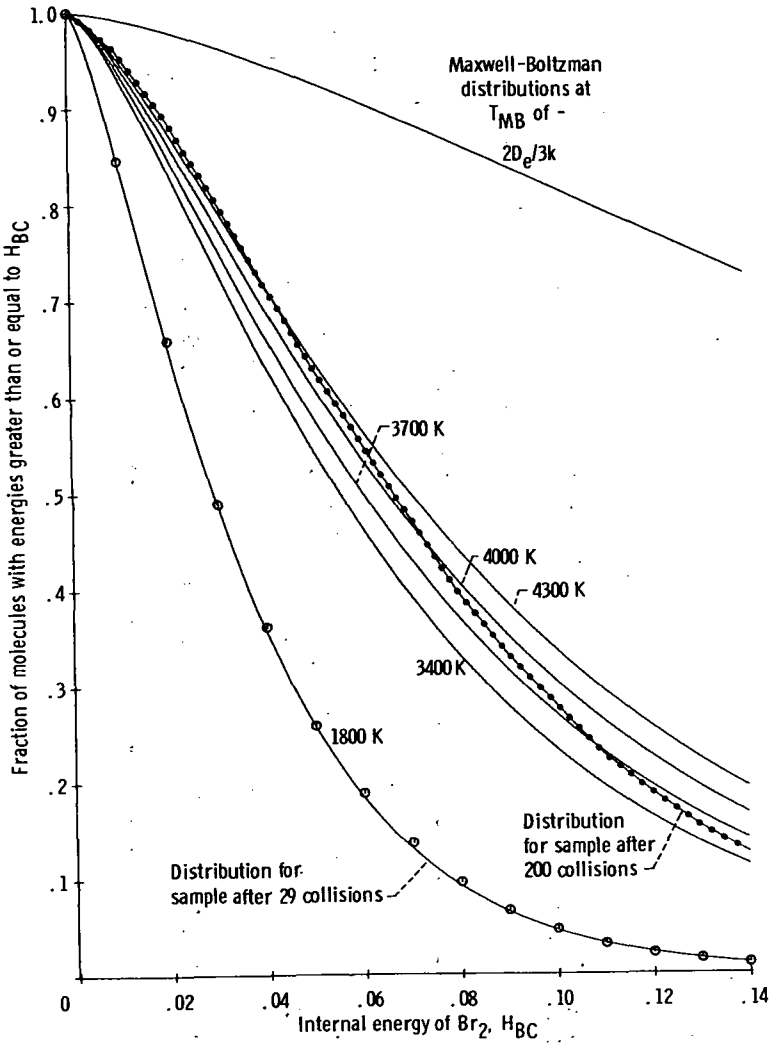


Figure 9. - Comparison of energy distribution for undissociated molecules in 10 000-molecule sample with required energy distributions for three-dimensional Maxwell-Boltzmann distributions.

bath temperature by roughly 100 K in this respect. As the system of diatomics evolves further toward dissociation, values of T_{MB} are considerably in excess of T_2, and the energy distribution again deviates strongly from a Maxwell-Boltzmann character. The spread in T_{MB} for the energy ranges $H_{BC} \geq 0.02$ u to $H_{BC} \geq 0.08$ u is 299 K after 70 collisions and 700 K after 200 collisions. Thus, we conclude that a system of vibrating rotators with internal energies initially distributed as a Maxwell-Boltzmann distribution, when embedded in a heat bath of inert gas atoms whose energies are also distributed as a Maxwell-Boltzmann distribution, will not evolve as a series of Maxwell-Boltzmann distributions at successively increasing values of T_{MB}, except instantaneously as T_{MB} passes through the heat-bath temperature. Hence, the system cannot be characterized by a temperature T_{MB} throughout the relaxation process.

Additional collisions to dissociation after H_{BC} reaches D_e	Number of occurrences
0	32
1 to 5	15
6 to 10	12
11 to 20	15
21 to 30	13
31 to 50	4
51 to 1000	0
1001 to 10 000	7
<25 000	2
	100

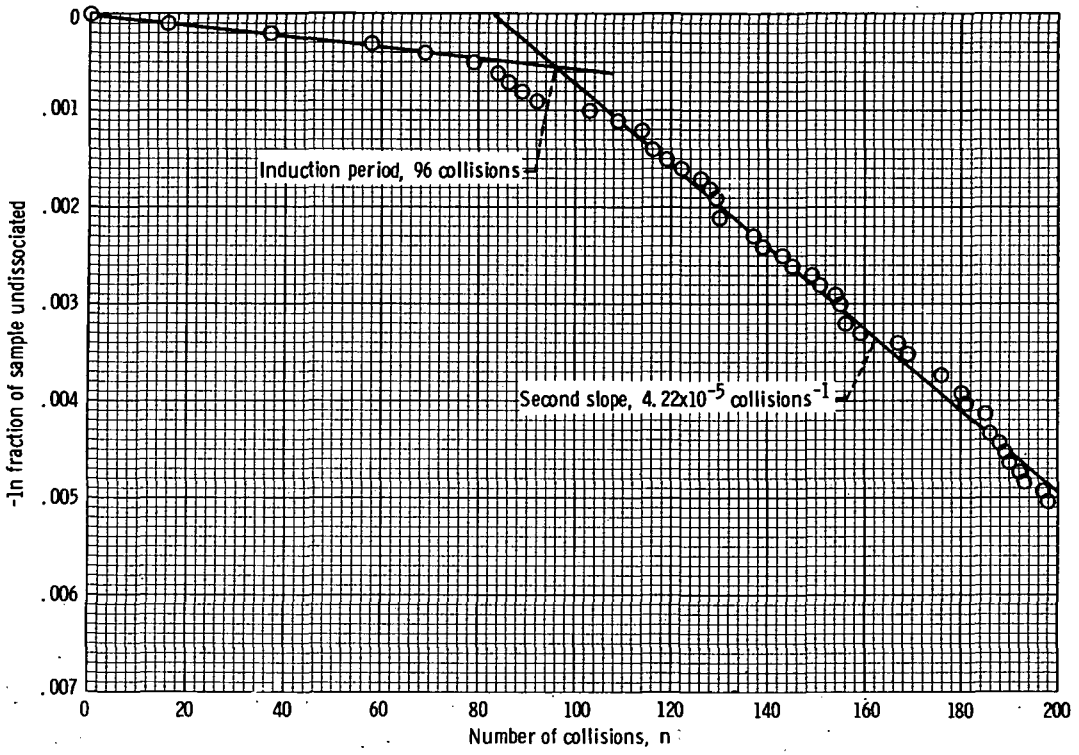


Figure 11. - Initial stage in dissociation of 10 000 Br_2 diatomics at preshocked-gas temperature T_1 of 300 K in Ar heat bath at shocked-gas temperature T_2 of 1800 K.

From these results it is seen that a molecule very commonly dissociates as soon as the internal energy reaches D_e, or shortly thereafter, but that a significant fraction of the molecules require many more collisions for dissociation.

Since there are many published theories of energy transfer and rate processes for diatomics that ignore rotation and vibration-rotation coupling, a special calculation was performed which attempts to evaluate the importance of these factors in the dissociation process. For this purpose a sample of 10 000 molecules, randomly selected at T_1 = 300 K, were allowed to undergo successive collisions to dissociation using only the five probability distributions in figure 5 for which $|\vec{M}_{BC}|^2(i) = 0$. The value of $|\vec{M}_{BC}|^2$ was set equal to zero after each collision, although $|\vec{M}_{BC}|^2$ was not really zero during

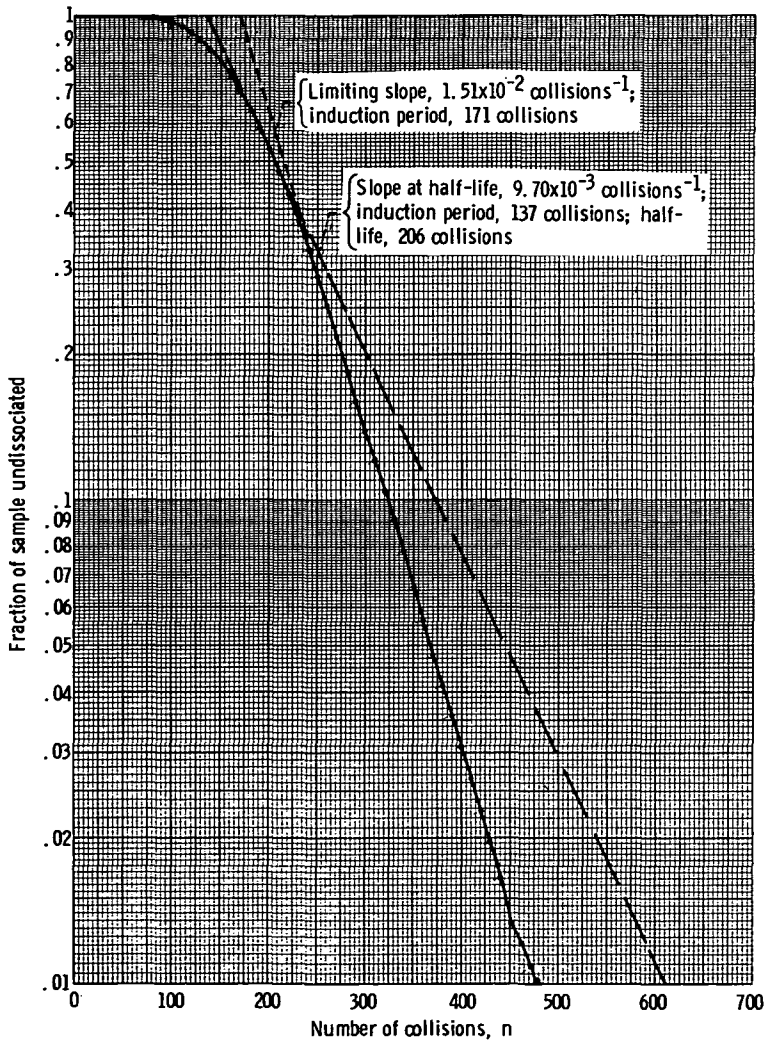


Figure 12. - Dissociation of 10 000 Br_2 diatomics with angular momentum defined to be zero with preshocked-gas temperature T_1 of 300 K in Ar heat bath at shocked-gas temperature T_2 of 1800 K.

a trajectory, and the assumption was made that dissociation would occur when $H_{BC} = 0.9999\ D_e$. Compared to collinear collision theories, this should correspond to the next more complicated collision model, where now the molecule is randomly oriented before each collision but the internal energy is still equated to the vibrational energy. A computer tabulation of the results is included in appendix E, and the resulting rate plot is shown in figure 12. Here the half-life is two orders of magnitude shorter than when angular momentum is included, being of the same order as the induction period. Thus, we conclude that including the influences of angular momentum and vibration-rotation coupling has a significant effect on the dissociation rate for the present system. On the other hand, a comparison of figures 11 and 12 indicates that the induction period is probably not as sensitive as the rate constant to the effects of rotation and vibration-rotation coupling, since the variation in τ is only 96 to 171.

Table V gives a summary of dissociation rates obtained from the slopes of figures 10 to 12 and by the use of equation (12) and compares these with the experimental rate given by equation (13). From this comparison it appears that calculations based on the present collision model, which assumes dissociation from the ground electronic state and classical motion, at best yield a rate 7.8 times greater than the published experimental rate at $T_2 = 1800$ K when the influence of rotation is included and a rate $\sim 10^3$ times greater when angular momentum is ignored. The values of K_D in table V are based on total

TABLE V. - SUMMARY OF MONTE-CARLO DISSOCIATION RATES

FOR Br_2 IN ARGON HEAT BATH AT 1800 K

Source of rate-determining slope	$\sigma_{Br_2, Ar}$			
	10 Å		3.589 Å	
	[a]$K_{D,calc}$	$K_{D,calc}/K_{D,exp}$	$K_{D,calc}$	$K_{D,calc}/K_{D,exp}$
Sample of 100 average 300 K molecules (fig. 10)				
Second slope	3.19×10^{11}	222	4.10×10^{10}	28.5
Limiting slope	1.97	137	2.54	17.6
Sample of 10 000 molecules at [b]$T_1 = 300$ K (fig. 11)				
Second slope	8.72×10^{10}	61	1.12×10^{10}	7.8
Sample of 10 000 molecules with [c]$\lvert\vec{M}_{BC}\rvert^2 \equiv 0$ (fig. 12)				
Slope at half-life	2.00×10^{13}	13 900	2.58×10^{12}	1710
Limiting slope	3.12	21 700	4.02	2790

[a]Where K_D is the specific rate constant for dissociation.
[b]Where T_1 is the preshocked-gas temperature.
[c]Where $\lvert\vec{M}_{BC}\rvert^2$ is angular momentum squared.

collision counts for $\rho = 10$ Å. If these were revised to a smaller value of $\rho = 6$ Å (see section on calculation of a dissociation rate), the values of K_D would be revised upward by a factor of 2.8.

DISCUSSION OF PRESENT MODEL IN RELATION TO THEORETICAL PRINCIPLES AND EXPERIMENT

In a recent paper Warshay compares the predictions of several models of rate processes to his experimental shock-tube measurements for the Br_2 dissociation in the presence of Ar, where the initial Br_2:Ar concentration ratio was 1:99 (ref. 1, fig. 2). These predictions are the dissociation models of Nielsen and Bak (ref. 10), Light (ref. 11), and Keck and Carrier (ref. 12) and the recombination models of Bunker and Davidson (ref. 13) and Benson, Fueno, and Berend (refs. 14 and 15). The assumption of microscopic reversibility permitted a conversion of recombination rates into dissociation rates by use of the equilibrium constant. In this section we will reflect on the results of the present work, and in a following discussion section we will compare our collision model and its results with some of these other theories.

As with all the other models in Warshay's comparison, it appears that the present model will predict a rate constant significantly higher than that of experiment. Consequently, either an error exists in the interpretation of the experimental data, or the present model for rate processes involves an energy transfer mechanism that is too efficient for the Br_2-Ar system.

The half-life of 4570 collisions (total collision count for $\rho = 10$ Å), predicted by the present model for Br_2 molecules at a heat-bath temperature of 1800 K, is equivalent to times of 0.44 and 3.4 microseconds (counted from $t = 0$) on the basis of the kinetic theory mean free time (eq. (11)) for $\sigma_{Br_2,Ar}$ of 10 and 3.589 Å, respectively. On the other hand, the experimental measurements for Br_2 concentration at 1827 K (ref. 4, fig. 3) can be plotted on a time scale of approximately 10^1 to 10^2 microseconds. The photomultiplier system used in these shock-tube measurements is quoted as having a "rate response" of 0.7 microsecond (ref. 16, p. 8). Our calculated half-life is thus close to the time constant for the electronic circuitry used in the experiments. Consequently, a dissociation rate as high as the one calculated could not be measured with that equipment.

A full test of the present model cannot be made with just one rate constant at one heat-bath temperature but would require at least two and possibly three heat-bath temperatures, as well as rates using other inert gases besides argon. For a given third body an Arrhenius plot of $\ln K_D$ against $1/T_2$ should show a temperature dependence

compatible with experiment, and at a given heat-bath temperature the experimental results indicate that K_D should be insensitive to the inert-gas species (ref. 1, fig. 3).

If we accept the interpretation of the experimental measurements as correct, we must then search for possible inadequacies in the collision model. An assessment of the effect of errors in the interaction potential (eqs. (4) and (5)) indicates that rather large errors in the potential constants should produce only minor effects on trajectories (ref. 2, footnote 21; ref. 3, pp. 11-12) except at heat-bath temperatures well below 1000 K, where $T_2 \approx \epsilon/k$. In addition, probability distributions for $\left(\Delta H_{BC}, \Delta\left|\vec{M}_{BC}\right|^2\right)$ have been shown to be both smoothly and slowly varying functions of heat-bath temperature above $T_2 = 1000$ K (ref. 3, p. 15). The largest effect on individual probability distributions for ΔH_{BC} and $\Delta\left|\vec{M}_{BC}\right|^2$ occurs when a change is made in the third body. An example of the change resulting in a single ΔH_{BC} probability distribution when helium is substituted for argon as the third body is shown in figure 13 (with potential constants taken from ref. 3, p. 11). The order-of-magnitude ranges for ΔH_{BC} changes

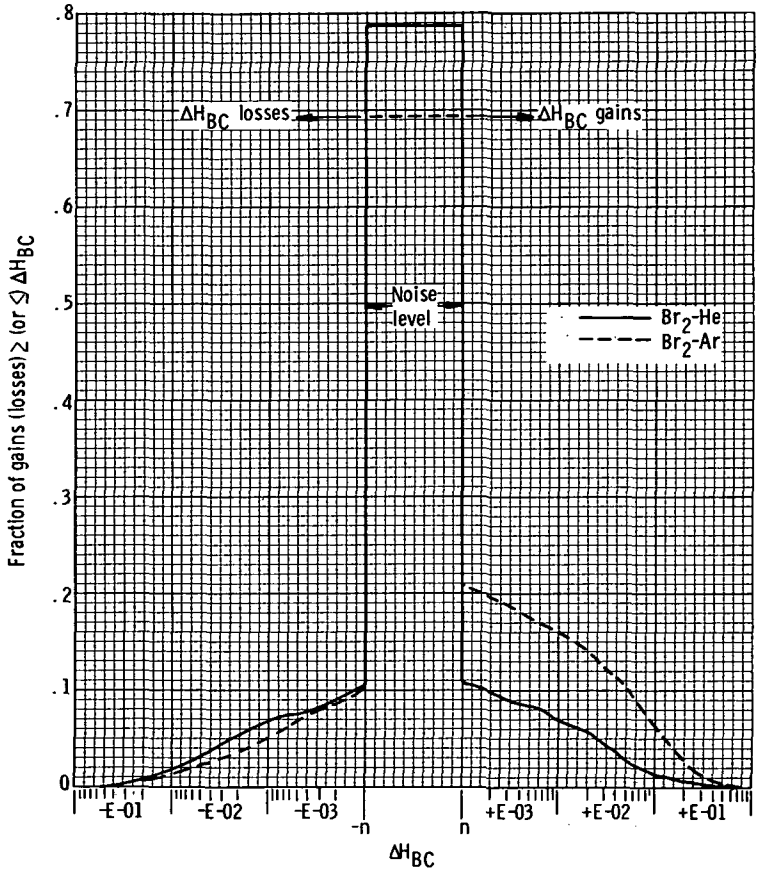


Figure 13. - Probability distributions for internal energy changes ΔH_{BC} per collision at shocked-gas temperature of 1800 K for set of initial molecule conditions ($H_{BC}(i) = 0.5\ D_e$, $\left|\vec{M}_{BC}\right|^2(i) = 0.1$), with Ar and He as third bodies.

are the same in both cases, the major change being in the relative population of energy increases. (Distributions for large $|\vec{M}_{BC}|^2(i)$ will show similar "gains" profiles but changed "losses" profiles.) An assessment of the sensitivities of $\left(\Delta H_{BC}, \Delta|\vec{M}_{BC}|^2\right)$ probability distributions to errors in potential constants, to heat-bath temperature, and to a change in the third body indicates that only the last of these is likely to lead to significant changes in probability distributions. It does not appear that sampling errors for initial atom energies could be serious enough to account for the discrepancy between theory and experiment. We also believe that the same is true for uncertainties in the values used for the potential constants.

If both the interpretation of experimental measurements and the collision model are basically correct, and if probable errors in the potential will not account for the discrepancy between the calculated and experimental rate constants, then a stabilization mechanism that will increase the average number of collisions to dissociation must be sought within the molecule itself. One idea that was investigated was that the assumption of dissociation involving only the $^1\sum_g^+$ ground state of Br_2 may be wrong. Bromine has an excited electronic state $^3\prod_{1(u)}$ which, like the ground state, is formed from two ground-state $Br\left(^2P_{3/2}\right)$ atoms, with both potentials coinciding at large $|\vec{R}_{BC}|$. Consequently, the question arises whether an almost dissociated molecule could cross over to the $^3\prod_{1(u)}$ state during a collision (i.e., when the atom is within the sphere of interaction), and then the free molecule lose energy by radiation back to the ground state before it encounters another atom (a transition which is allowed). Emission between the excited and ground electronic states of Br_2 in the presence of argon has been studied in shock-tube experiments by Palmer (ref. 17) and at low pressure by Clyne and Coxon (ref. 18). These transitions give rise to an emission spectrum in the red to infrared. Such radiation mechanism, if it could occur efficiently, would stabilize the diatomics and hence decrease the probability that a ground-state molecule near dissociation would actually dissociate. Upon further investigation, however, such a process was discounted as a possible stabilization mechanism for the reason that the radiative lifetimes of these excited states (under the experimental conditions) are many times that of t_{mf} ($\sim 10^{-8}$ sec). Hence, even if a molecule were to enter the $^3\prod_{1(u)}$ state, it would probably be dissociated by further collisions long before it could radiate. On the other hand, a stabilization mechanism by radiation that would lower K_D by an order of magnitude would require a radiative lifetime less than or of the order of t_{mf}.

We thus arrive at the conclusion that a stabilization mechanism for the diatomics must be sought within the $^1\sum_g^+$ ground state itself. From what has already been ruled out, it appears that a remaining possibility is that the classical vibration-rotation coupling provides an energy transfer mechanism that is too efficient. It was originally thought that Br_2 might provide an optimum system where classical mechanics would be

applicable to the internal energy modes of the molecule, because of the fact that the $^1\sum_g^+$ ground state consists of a large number of closely spaced vibrational levels (refs. 2 and 3). It now appears that such a criterion for the strict applicability of classical mechanics may not be entirely accurate. As a tentative hypothesis, a semiclassical theory where vibration and rotation are allowed to couple only in energy increments that could lead to "quantum jumps" in vibrational energy might be considered, with permitted vibrational energies distributed in a level structure like that of a quantum mechanical anharominc oscillator. If such level structure for the molecule could be incorporated into the theory, it may provide a needed stabilization mechanism without the necessity of either assuming that vibration-rotation coupling does not exist or that collision orientations are unrealistically restricted (as, e.g., in collinear collision theories). An assessment of the practicality of such a scheme, however, must await the outcome of further research.

DISCUSSION OF RELATED WORK AND THEORETICAL CONCEPTS

We will now compare our collision model and its results with several other collision theories. In these discussions we will not consider the recombination theories in Warshay's comparison (refs. 13 to 15) since, despite some approximate physical arguments to the contrary, there are questions regarding the validity of the often assumed equilibrium constant relation between dissociation and recombination rates (ref. 19) that have so far not been satisfactorily answered.

Comparison of Present Model with Other Theories

Of the three dissociation models that Warshay compared with his experiments (ref. 1), that of Keck and Carrier (ref. 12) comes closest to the present model with regard to the factors it attempts to take into account. Theirs is a master-equation approach to a "diffusion theory" where a system of oscillators is allowed to undergo vibrational relaxation in a heat bath of inert-gas atoms and the coupled vibration, dissociation, and recombination is studied. Their definition of conditions at time zero differs from ours in that they assume equilibrium in translational and rotational degrees of freedom. (This should not be of consequence for a rate calculation if vibration-rotation coupling is not severe, but it could make a difference in a description of the initial stage of a system evolution.) In the dissociation process they treat the total internal energy of the molecule as a coordinate, where diffusion takes place with respect to the total internal energy required to dissociate a molecule with a given angular momentum. As these

authors recognize, however, this does not adequately treat the problem of the influence of rotation (and, of course, vibration-rotation interaction) in the relaxation process (ref. 20, p. 1895). A graphical extrapolation of the Arrhenius plot in figure 2 of reference 1 for the Keck and Carrier theory to the heat-bath temperature 1800 K gives a value for K_D nearly identical to that obtained in the present calculation from the limiting slope for the sample of 100 molecules with $\sigma_{Br_2,Ar} = 3.589$ Å (table V). Of all the theories in Warshay's comparison, the Keck-Carrier theory also predicts no variation in K_D with a change in the third body and, hence, comes the closest to experiment in that regard.

The present dissociation model is somewhat similar to the Keck and Carrier theory, except that no type of master equation is assumed for the system evolution. The evolution process is instead a natural outcome of a Monte-Carlo interpolation scheme. We start out with the basic microscopic concept of an atom-molecule collision, with random orientation and the atoms picked at random from a heat bath, and build up a model for the macroscopic system as it evolves in time by Monte-Carlo averaging. Our model is more complicated, however, in that it does not insert any restriction on the internal motion of the molecule, other than that it is classical and of pairwise additivity of atom-molecule forces. Hence, the present model takes full account of the influence of both vibration and rotation in the relaxation process.

The Keck and Carrier theory predicts some nonequilibrium in the population of upper vibrational levels of the molecules due to effects of dissociation and recombination. (See, e.g., ref. 21, p. 2251, for a discussion of the Keck and Carrier theory.) Our calculations, on the other hand, lead to nonequilibrium effects more severe than any reported for the Keck and Carrier theory. The present results for the sample of 10 000 molecules which was allowed to undergo 200 collisions from time zero predict a substantial nonequilibrium population for all energy levels before dissociation (and, hence, recombination) even become important. For a system of molecules in equilibrium with the heat bath at T_2, internal energies should be distributed according to the Boltzmann factor $\exp(-H_{BC}/kT_2)$. Thus, if a collection of molecules at time zero with internal energies distributed according to the proportionality factor $\exp(-H_{BC}/kT_1)$ is embedded in a heat bath at T_2, we might expect the system to undergo a relaxation and finally arrive at a state where internal energies are distributed according to a Maxwell-Boltzmann distribution at heat-bath temperature T_2. In an equilibrium heat bath at T_2, this distribution should be maintained indefinitely thereafter, so long as a significant fraction of the molecules has not been lost to dissociation. However, from figures 8 and 9 it appears that this is not the case. After only 29 collisions, internal energies pass right through an energy distribution that could reasonably be thought to constitute a thermodynamic equilibrium with the heat bath. At this point, however, the initial transient (fig. 7) has hardly even begun to subside. From the computer printout for the

sample of 10 000 molecules (appendix E), we find that after 200 collisions (where 9950 out of 10 000 molecules remain undissociated) the average internal energy of the undissociated molecules is 0.07658 u = 0.240 D_e. If this were the average internal energy of an equilibrium sample ((3/2)kT), the corresponding temperature would be 3699 K - more than twice the heat-bath temperature. However, a closer examination of the energy distribution after 200 collisions in figure 9 reveals that the sample distribution after 200 collisions also deviates strongly from the required shape for a Maxwell-Boltzmann distribution, being too heavily populated at low energies and too sparsely populated at high energies. This nonequilibrium behavior after 29 collisions is rather surprising and perhaps warrants a more detailed study. The fact must be kept in mind, regarding this nonequilibrium, that all the probability distributions (appendix F) that were used in the calculation were determined for conditions where the relative translational energies of all species were at equilibrium at T_2. Hence, before a significant fraction of the sample has dissociated, it is not possible to argue either on the basis of a depletion of the sample due to dissociation or from the point of view that recombination is being ignored.

The theory of Nielsen and Bak (ref. 10) treats the diatomic as a harmonic oscillator composed of two hard spheres embedded in a hard-sphere monatomic gas. The hard-sphere interaction implies impulsive energy transfer and permits a large transfer of energy to the vibrational motion. A separation of rotational and vibrational motion is effected in the process of performing an integration over rotational coordinates of the molecule, by regarding the molecule as a rigid rotator (ref. 10, p. 669). Nielsen and Bak also assume equilibrium in the various degrees of freedom before collision. As they point out (ref. 10, pp. 671-672), the approximation of an impulsive interaction would be expected to give a more adequate description of energy transfer when internal motions in the molecule are slow compared to relative translational motion and, hence, at high heat-bath temperatures. In the present case these conditions are not always fulfilled, however. Although energy transfer can be regarded as approximately impulsive (ref. 3, pp. 10-11 and 20), this cannot be construed as a pure vibrational or pure rotational excitation. In addition, circular velocities of rotational motion - especially near dissociation - are likely to be comparable to relative translational velocities (table III).

Of the three dissociation theories considered by Warshay, that of Light (ref. 11) involved assumptions that are the most completely at odds with features of the collision process found to be important in the present model. Light's theory is an adiabatic scattering approach to dissociation, which involves an expansion of the Liouville equation in powers of the reciprocal of the oscillator frequency. The model assumes both adiabatic collisions with neglect of rotational energy of the oscillator and net energy transfer only upon dissociation. Hence, this model is not capable of describing relaxation processes.

Comparison of Initial Stage in Evolution with Predictions of Other Theories

The evolution problem studied herein (figs. 7 to 9) has a bearing on the significance of various assumptions in relaxation theories for physical conclusions. For example, in studying the vibrational and rotational relaxation of a system of rotating oscillators, Herman and Shuler (ref. 8) assumed a rigid rotator - harmonic oscillator model for a molecule, without any vibration-rotation interaction. They furthermore assumed that rotational degrees of freedom are in equilibrium with the heat bath and, hence, could be neglected in vibrational relaxation. They concluded that both vibrational and rotational relaxation should occur from an initial Boltzmann distribution to a final Boltzmann distribution through a sequence of intermediate Boltzmann distributions and that rotation can be considered to relax independently of vibration. (However, in the same paper (ref. 8, p. 373) the authors note a large discrepancy between theory and experiment for the dissociation of I_2 and Br_2.) In an earlier paper of the same series (ref. 22) the conclusion was also drawn that neglect of anharmonicity in the oscillators should not lead to serious errors, and in reference 8 it is speculated that the same is probably true of the neglect of centrifugal stretching and vibration-rotation interaction. Such a conclusion may be in doubt, however, in view of the fact that "diffusion theory" calculations of Brau, Keck, and Carrier for dissociation (even though not accounting for vibration-rotation effects) indicate that anharmonicity in the oscillator introduces some nonequilibrium effects at all vibrational energies (ref. 20, p. 1894). In view of the significant non-Boltzmann-like relaxation obtained with the present model with vibration-rotation coupling included, it appears that earlier theoretical predictions of Boltzmann-like relaxation processes may have followed largely from the nature of the simplifying assumptions that were built into these theories.

Lewis Research Center,
National Aeronautics and Space Administration,
Cleveland, Ohio, August 22, 1972,
502-04.

APPENDIX A

SYMBOLS

Å	scaled unit of length, 10^{-10} meter
b	impact parameter
D_e	dissociation energy for Br_2 ground state, 0.31916 u
D_j	potential constants for Br-Br interaction, $\sum_1^3 D_j = D_e$ where $D_1 = 0.31801$ u; $i = \sqrt{-1}$ $\begin{cases} D_2 = 0.57547\times10^{-3} - i0.88651\times10^{-3} \text{ u} \\ D_3 = 0.57547\times10^{-3} + i0.88651\times10^{-3} \text{ u} \end{cases}$
E	computer symbol for exponent to base 10; example: 0.0040 = 0.40 E-02
F_i	function constructed from trajectory calculations that associates a choice of three random numbers with a pair $\left(\Delta H_{BC}, \Delta\lvert\vec{M}_{BC}\rvert^2\right)$
H	Hamiltonian (total energy)
H_A	relative kinetic energy of Br_2-Ar motion
H_{ABC}	energy of relative motion of particles A, B, and C
H_{BC}	internal energy of Br_2
H_{CM}	kinetic energy of translation of Br_2-Ar center of mass
H_r	rotational energy
H_v	vibrational energy
H_v(p-p)	peak-to-peak amplitude in H_v at constant H_{BC} due to vibration-rotation coupling
$\hbar^2$	Planck's constant squared divided by $4\pi^2$, 0.111197×10^{-3} u^2t^2
$\vec{i}_{ij}$	unit vector
J	rotational quantum number
K_D	specific rate constant for dissociation, cm^3/(mole)(sec)
k	Boltzmann's constant, 0.138054×10^{-4} uK^{-1}
$\vec{M}$	angular momentum about A-B-C center of mass

$\lvert\vec{M}\rvert^2$	(with or without subscripts), angular momentum squared, $m^2 \text{Å}^2 v^2$
$\vec{M}_{BC}$	angular momentum about Br_2 center of mass
m	scaled unit of mass, 10^{-26} kg; subscripts indicate masses of particles
N	number of atoms per cubic centimeter
n	number of collisions
$\vec{P}$	relative Br_2-Ar momentum
$\vec{P}_{BC}$	momentum of particle B relative to particle C
p_j	set of initial molecule conditions for which a probability distribution for $\left(\Delta H_{BC}, \Delta\lvert\vec{M}_{BC}\rvert^2\right)$ was determined
$\vec{R}_{BC}$	location of particle B relative to particle C; similar definitions for $\vec{R}_{AB}$ and $\vec{R}_{AC}$
$\lvert\vec{R}_{BC}(e)\rvert$	equilibrium internuclear separation for Br_2 ground state, 2.28161 Å
T	temperature, kelvin; used with or without subscripts
T_{MB}	temperature corresponding to a three-dimensional Maxwell-Boltzmann energy distribution
T_1	preshocked-gas temperature, 300 K in present calculations
T_2	heat-bath (shocked gas) temperature, 1800 K in present calculations
t	scaled unit of time, 10^{-14} sec
t_{mf}	kinetic theory mean free time
u	scaled unit of energy, 10^{-18} joule, (1 joule = 10^7 ergs = $[6.241(97)\pm(12)]\times10^{18}$ eV = $[5.034(80)\pm(18)]\times10^{22}$ cm^{-1} = $[1.4399(8)\pm(4)]\times10^{20}$ kcal/mole)
$V_1\left(\lvert\vec{R}_{BC}\rvert\right)$	interaction potential for Br-Br
$V_2\left(\lvert\vec{R}_{AB}\rvert\right)$, $V_2\left(\lvert\vec{R}_{AC}\rvert\right)$	atom-molecule interaction potentials
v	scaled unit of velocity, 10^4 meters/sec
$\vec{X}$	location of Ar relative to Br_2 center of mass
x	degree of dissociation

Z — symbol for random number in the interval [0, 1] (with or without subscripts)

$\bar{Z}_{Br_2,Ar}$ — in kinetic theory: hard-sphere collision frequency for a Br_2 molecule in a heat bath of Ar atoms; in present theory: frequency with which an Ar atom comes within a distance of the Br_2 center of mass equal to the effective radius of the molecule

α_j — potential constants in Br-Br interaction, V_1

$$\alpha_1 = 1.9756 \text{ Å}^{-1}$$

$$i = \sqrt{-1} \quad \begin{cases} \alpha_2 = 1.5994 + i6.4990 \text{ Å}^{-1} \\ \alpha_3 = 1.5994 - i6.4990 \text{ Å}^{-1} \end{cases}$$

ϵ — Lennard-Jones potential constant in V_2, 0.3411×10^{-2} u

Θ — longitude in cylindrical coordinates

θ — colatitude in spherical polar coordinates

μ_{BC} — reduced mass of Br_2 molecule, 6.63420 m

$\mu_{A,BC}$ — reduced mass of Br_2-Ar system, 5.30667 m

ρ — radius of sphere of interaction (10 Å in present calculations)

σ — Lennard-Jones potential constant in V_2, 3.867 Å

$\sigma_{Br_2,Ar}$ — kinetic theory separation of centers for hard spheres on impact, or sphere of interaction in present collision model

τ — induction period defined as time after $t = 0$ where the initial and second slopes of a rate plot intersect

$\dot{\Phi}$ — instantaneous angular velocity in plane of rotation

φ — longitude in spherical polar coordinates

Special symbols:

[ ] — concentration, when enclosing a symbol for a chemical element or molecule

⟨ ⟩ — average value

APPENDIX B

INTERPOLATION METHOD

Problem Statement

In carrying out the Monte-Carlo calculations, it is necessary to find ΔH_{BC} and $\Delta|\vec{M}_{BC}|^2$ for any initial values $H_{BC}(i)^*$ and $|\vec{M}_{BC}|^2(i)^*$ and for any three random numbers Z_1^*, Z_2^*, and Z_3^*. This problem can be viewed as two two-dimensional interpolation problems as follows. Let the set of 30 initial values of $H_{BC}(i)$ and $|\vec{M}_{BC}|^2(i)$, for which probability distributions have been developed, be denoted by

$$p_j = \left\{ \left[H_{BC}(i) \right]_j , \left[|\vec{M}_{BC}|^2(i) \right]_j \right\}_{j=1}^{30}$$

For any choice of Z_1, Z_2, and Z_3, we can use the probability distributions to calculate $\left(\Delta H_{BC}\right)_j$ and $\left(\Delta|\vec{M}_{BC}|^2\right)_j$ for any value of j from 1 to 30.

Hence, to find ΔH_{BC}^* at the arbitrary point, we can interpolate between points p_j in the $\left(H_{BC}(i), |\vec{M}_{BC}|^2(i)\right)$ plane. Similarly, we can interpolate between the points p_j to find $\Delta|M_{BC}|^{2^*}$.

Outline of Interpolation Method

The interpolation method consists of the following six steps:

(1) Pick several points from p_j that surround the arbitrary point, $\left(H_{BC}(i)^*, |\vec{M}_{BC}|^2(i)^*\right)$, in the $\left(H_{BC}, |\vec{M}_{BC}|^2\right)$ plane. This process will be referred to as bracketing. (For further details see next section Discussion of Bracketing Method.)

(2) Using the probability distributions, find ΔH_{BC} and $\Delta|\vec{M}_{BC}|^2$ at each of the bracketing points for the chosen Z_1^*, Z_2^*, and Z_3^*.

(3) Find a plane, $\Delta H_{BC} = a_H(H_{BC}) + b_H\left(|\vec{M}_{BC}|^2\right) + c_H$, in $\left(H_{BC}, |\vec{M}_{BC}|^2, \Delta H_{BC}\right)$ space that is a good fit at the bracketing points to the corresponding ΔH_{BC} found in 2. (For further details see section Discussion of Plane Fitting.)

(4) Assume that ΔH_{BC} at the arbitrary point lies on the plane found in 3. That is, let $\Delta H^*_{BC} = a_H(H^*_{BC}) + b_H\left(|\vec{M}_{BC}|^{2*}\right) + c_H$.

(5) Find a plane, $\Delta|\vec{M}_{BC}|^2 = a_M(H_{BC}) + b_M\left(|\vec{M}_{BC}|^2\right) + c_M$, in $\left(H_{BC}, |\vec{M}_{BC}|^2, \Delta|\vec{M}_{BC}|^2\right)$ space that is a good fit at the bracketing points to the corresponding $\Delta|\vec{M}_{BC}|^2$ found in 2.

(6) As in 4, let $\Delta|\vec{M}_{BC}|^{2*} = a_M(H^*_{BC}) + b_M\left(|\vec{M}_{BC}|^{2*}\right) + c_M$.

Discussion of Bracketing Method

To bracket a given point $\left(H^*_{BC}, |\vec{M}_{BC}|^{2*}\right)$ we attempt to find four points, p_{LL}, p_{LH}, p_{HL}, and p_{HH}, from p_j as follows:

(1) p_{LL} has a lower H_{BC} and a lower $|\vec{M}_{BC}|^2$ than $\left(H^*_{BC}, |\vec{M}_{BC}|^{2*}\right)$.

(2) p_{LH} has a lower H_{BC} and a higher $|\vec{M}_{BC}|^2$ than $\left(H^*_{BC}, |\vec{M}_{BC}|^{2*}\right)$.

(3) p_{HL} has a higher H_{BC} and a lower $|\vec{M}_{BC}|^2$ than $\left(H^*_{BC}, |\vec{M}_{BC}|^{2*}\right)$.

(4) p_{HH} has a higher H_{BC} and a higher $|\vec{M}_{BC}|^2$ than $\left(H^*_{BC}, |\vec{M}_{BC}|^{2*}\right)$.

The points p_j were chosen to cover that part of the $\left(H_{BC}, |\vec{M}_{BC}|^2\right)$ plane that represents undissociated molecules. Hence, it is usually possible to bracket a point representing an undissociated molecule by three or four points from p_j. Near dissociation it is sometimes possible to bracket by only two points.

Discussion of Plane Fitting

If we have found three bracketing points, then there is a unique plane over $\left(H_{BC}, |\vec{M}_{BC}|^2\right)$ space that takes on the values ΔH_{BC} $\left(\text{or } \Delta|\vec{M}_{BC}|^2\right)$ corresponding to the three points. If there are four bracketing points, then, in general, there will be no plane that takes on the values of ΔH_{BC} $\left(\text{or } \Delta|\vec{M}_{BC}|^2\right)$ at all four points. In this case we choose a plane according to the least-squares criteria. That is, we choose that plane which minimizes the sum of the squares of the four residuals. A residual at a bracketing point is the difference between the ΔH_{BC} $\left(\text{or } \Delta|\vec{M}_{BC}|^2\right)$ calculated from the probability distributions and the ΔH_{BC} or $\left(\Delta|\vec{M}_{BC}|^2\right)$ calculated from the plane equation. (This ignores any curvature that might be taken into account in some four-point interpolation schemes (ref. 23, ch. 25). From an inspection of individual F_i (appendix F), we have concluded that bracketing probability distributions usually lead

to four $\left(\Delta H_{BC},\ \Delta\left|\vec{M}_{BC}\right|^2\right)$ pairs that are similar enough for any curvature to be ignored.)

If only two bracketing points exist, we do not fit a plane but simply do a one-dimensional linear interpolation on H_{BC}.

APPENDIX C

SELECTION OF INITIAL CONDITIONS

The general formula for a Maxwell-Boltzmann distribution is given by

$$dw = \left[\frac{1}{\Gamma(s+1)}\right]\left(\frac{H}{kT}\right)^{s} \exp\left(\frac{-H}{kT}\right)\left(\frac{dH}{kT}\right) \tag{C1}$$

where Γ is a gamma function, and where $s = 1/2$ corresponds to a three-dimensional distribution or a two-dimensional flux distribution, while $s = 1$ corresponds to a three-dimensional flux distribution (ref. 24). For calculating probability distributions for $\left(\Delta H_{BC}, \Delta|\vec{M}_{BC}|^2\right)$ changes, given H_{BC} and $|\vec{M}_{BC}|^2$, an atom had to be selected from a three-dimensional flux distribution corresponding to T_2, since only atoms moving toward the molecule are of interest (see fig. 1). That is, the range of $\dot{X}_3$ is 0 to ∞. Since definite values for $H_{BC}(i)$ and $|\vec{M}_{BC}|^2(i)$ were always specified for such calculations, the position and velocity vectors for the molecule had only to be randomly oriented over a sphere before we proceeded with the integration of the equations of motion. Formulas for choosing appropriate initial conditions are derived in references 2 and 3. Their derivations are not repeated here, but the results are listed for convenience.

For the atom, cylindrical coordinates for $\dot{\vec{X}}$ are introduced by

$$\left.\begin{aligned} \dot{X}_1 &= |\dot{\vec{X}}|_{1,2} \cos\Theta \\ \dot{X}_2 &= |\dot{\vec{X}}|_{1,2} \sin\Theta \\ \dot{X}_3 &= \vec{i}_3 \cdot \dot{\vec{X}} \end{aligned}\right\} \tag{C2}$$

and initial conditions are picked by

$$\left.\begin{aligned} \dot{X}_1 &= \left(\frac{-2 \ln Z_{1,2}}{\beta_2 \mu_{A,BC}}\right)^{1/2} \cos(2\pi Z_\Theta) \\ \dot{X}_2 &= \left(\frac{-2 \ln Z_{1,2}}{\beta_2 \mu_{A,BC}}\right)^{1/2} \sin(2\pi Z_\Theta) \\ \dot{X}_3 &= \left(\frac{-2 \ln Z_3}{\beta_2 \mu_{A,BC}}\right)^{1/2} \end{aligned}\right\} \tag{C3}$$

where Z_Θ, $Z_{1,2}$, and Z_3 are random numbers uniformly distributed in the interval $[0, 1]$, and $\beta_2 = 1/kT_2$. If initial conditions for many atoms are picked in this way, initial kinetic energies $H_A(i)$ will be distributed according to a Maxwell-Boltzmann flux distribution at heat-bath temperature T_2 (ref. 2, table I; and ref. 3, table I).

Given H_{BC} and $|\vec{M}_{BC}|^2$, the orientation of $\vec{R}_{BC}$ is randomly distributed over a sphere by introducing spherical polar coordinates

$$\left.\begin{aligned} R_{BC,1} &= |\vec{R}_{BC}| \sin\theta \cos\varphi \\ R_{BC,2} &= |\vec{R}_{BC}| \sin\theta \sin\varphi \\ R_{BC,3} &= |\vec{R}_{BC}| \cos\theta \end{aligned}\right\} \tag{C4}$$

and with $|\vec{R}_{BC}|(i) = |\vec{R}_{BC}(e)|$, choosing φ and θ by

$$\left.\begin{aligned} \varphi &= 2\pi Z_\varphi \\ \theta &= \cos^{-1}(1 - 2Z_\theta) \end{aligned}\right\} \tag{C5}$$

where Z_φ and Z_θ are random numbers. For velocity components (with $V_1(i) = 0$), $|\dot{\vec{R}}_{BC}|(i)$ is calculated from $\frac{1}{2}\mu_{BC}|\dot{\vec{R}}_{BC}|^2 = H_v$ and a $\pm$ sign is affixed to the result. A plane of rotation is selected by choosing

$$|\dot{\theta}| = |\dot{\Phi}|Z \tag{C6}$$

where Z is a random number and

$$|\dot{\Phi}| = \left| \left(\frac{2H_r}{\mu_{BC}} |\vec{R}_{BC}(e)|^2 \right)^{1/2} \right|$$

is the magnitude of the instantaneous angular velocity in the plane of rotation, and a $\pm$ sign is randomly affixed to $|\dot{\theta}|$. Finally $|\dot{\varphi}|$ is calculated from

$$\dot{\varphi}^2 = \frac{\dot{\Phi}^2 - \dot{\theta}^2}{\sin^2\theta} \tag{C7}$$

and a $\pm$ sign is randomly affixed to the result.

For determining a dissociation rate, molecules at time zero are selected at random from a three-dimensional Maxwell-Boltzmann distribution at temperature T_1 and are allowed to undergo successive collisions to dissociation under the conditions of the heat-bath temperature T_2. Initial conditions for the molecule must correspond to a full three-dimensional distribution, not a three-dimensional flux as with the atom, because for the molecule the range of all velocity components $\dot{R}_{BC,j}$ $(j = 1, 2, 3)$ is $-\infty$ to $+\infty$. Since probability distributions for $\left(\Delta H_{BC}, \Delta|\vec{M}_{BC}|^2\right)$ changes per collision have already been determined for a random orientation of the molecule, initial conditions for the purpose of interpolation do not have to be determined as if the equations of motion were to be integrated. That is, only initial values for H_{BC} and $|\vec{M}_{BC}|^2$ need be picked at T_1, but no random orientation of position and velocity vectors is needed.

The derivation of initial conditions for $\dot{\vec{R}}_{BC}$ is very similar to that used for $\dot{\vec{X}}$, except that the $\dot{R}_{BC,3}$ component ranges from $-\infty$ to $+\infty$. As with $\dot{\vec{X}}$, the problem can be handled by introducing cylindrical coordinates

$$\left.\begin{aligned} \dot{R}_{BC,1} &= |\dot{\vec{R}}_{BC}|_{1,2} \cos\Theta \\ \dot{R}_{BC,2} &= |\dot{\vec{R}}_{BC}|_{1,2} \sin\Theta \\ \dot{R}_{BC,3} &= \vec{i}_3 \cdot \dot{\vec{R}}_{BC} \end{aligned}\right\} \tag{C8}$$

so that the distribution for $\dot{\vec{R}}_{BC}$ is

$$f d\dot{\bar{R}}_{BC} = \mathcal{N} \exp\left[-\frac{1}{2}\beta_1 \mu_{BC}\left(\left|\dot{\bar{R}}_{BC}\right|^2_{1,2} + \dot{R}^2_{BC,3}\right)\right] \left|\dot{\bar{R}}_{BC}\right|_{1,2} d\left|\dot{\bar{R}}_{BC}\right|_{1,2} d\Theta \, d\dot{R}_{BC,3} \tag{C9}$$

where $\beta_1 = 1/kT_1$ and $\mathcal{N}$ is a normalization factor. From here the derivation for the 1 and 2 components of $\dot{\bar{R}}_{BC}$ proceeds like the derivation for $\dot{X}_1$ and $\dot{X}_2$ (refs. 2 and 3), yielding

$$\left.\begin{aligned} \dot{R}_{BC,1} &= \left(\frac{-2 \ln Z_{ij}}{\beta_1 \mu_{BC}}\right)^{1/2} \cos(2\pi Z_\Theta) \\ \dot{R}_{BC,2} &= \left(\frac{-2 \ln Z_{ij}}{\beta_1 \mu_{BC}}\right)^{1/2} \sin(2\pi Z_\Theta) \end{aligned}\right\} \tag{C10}$$

where Z_{ij} and Z_Θ are random numbers. (If eqs. (C2) and (C10) are used at the same time, different random numbers Z_Θ should be chosen for each set of formulas.) The distribution for $\dot{R}_{BC,3}$ is handled by the "direct method" (ref. 23, p. 953). Let

$$g = \left(\beta_1 \mu_{BC}\right)^{1/2} \dot{R}_{BC,3} \tag{C11}$$

Then

$$\exp\left(-\frac{1}{2}\beta_1 \mu_{BC} \dot{R}^2_{BC,3}\right) d\dot{R}_{BC,3} \rightarrow \exp\left(\frac{-g^2}{2}\right) dg \xrightarrow[(-\infty \text{ to } +\infty)]{\text{normalized}} \left(\frac{1}{\sqrt{2\pi}}\right) \exp\left(\frac{-g^2}{2}\right) dg \tag{C12}$$

so that the cumulative distribution is

$$\left(\frac{1}{\sqrt{2\pi}}\right) \int_{-\infty}^{g} \exp\left(\frac{-g^2}{2}\right) dg \tag{C13}$$

According to the "direct method" we must pick a pair of values for g by

$$g_a = \left(-2 \ln Z_a\right)^{1/2} \cos(2\pi Z_b)$$

$$g_b = \left(-2 \ln Z_a\right)^{1/2} \sin(2\pi Z_b)$$

where Z_a and Z_b are random numbers, or in terms of $\dot{R}_{BC,3}$,

$$\dot{R}_{BC,3} = \left(\frac{-2 \ln Z_a}{\beta_1 \mu_{BC}}\right)^{1/2} \begin{cases} \cos(2\pi Z_b) \\ \\ \sin(2\pi Z_b) \end{cases} \tag{C14}$$

Initial values for $\dot{R}_{BC,3}$ are selected in successive picks by alternating between $\cos(2\pi Z_b)$ and $\sin(2\pi Z_b)$.

For present purposes we have taken $|\vec{R}_{BC}|(i) = |\vec{R}_{BC}(e)|$ and $|\dot{\vec{R}}_{BC}|(i) = \left|\left(-2 \ln Z_{ij}/\beta_1 \mu_{BC}\right)^{1/2}\right|$, where $\frac{1}{2}\mu_{BC}|\dot{\vec{R}}_{BC}|^2$ must not be greater than $0.999\ D_e$ in order to avoid choosing a starting molecule with an internal energy exceeding that corresponding to data sets for $0.999\ H_{BC,max}$. This corresponds to a random number in the range $0 \le Z_{ij} \le e^{-62.01}$, which has a negligible chance of ever being chosen on a random-number generator. Thus, in the rare event that a random number in this range should be chosen, that choice can be discarded without affecting statistical results.

The square of the angular momentum for the molecule is given by

$$|\vec{M}_{BC}|^2 = \left(R_{BC,2}P_{BC,3} - R_{BC,3}P_{BC,2}\right)^2 + \left(R_{BC,3}P_{BC,1} - R_{BC,1}P_{BC,3}\right)^2 + \left(R_{BC,1}P_{BC,2} - R_{BC,2}P_{BC,1}\right)^2 \tag{C15}$$

where $\vec{P}_{BC} = \mu_{BC}\dot{\vec{R}}_{BC}$. In the present instance it is only necessary to pick a magnitude for angular momentum, and not the orientation, so that it is sufficient to take $R_{BC,1} = R_{BC,2} = 0$, $R_{BC,3} = |\vec{R}_{BC}(e)|$, giving

$$|\vec{M}_{BC}|^2(i) = \left(-R_{BC,3}P_{BC,2}\right)^2 + \left(R_{BC,3}P_{BC,1}\right)^2 \tag{C16}$$

At the temperature $T_1 = 300$ K, $kT_1 = 0.013\ D_e$, whereas the zero RKR vibrational level for the ground state of the Br_2 molecule corresponds to 0.010 De (ref. 3, table II). This corresponds to classical turning points for the vibrational motion of $|\vec{R}_{BC}|_{max} = 2.3347$ Å and $|\vec{R}_{BC}|_{min} = 2.2325$ Å, so that $|\vec{R}_{BC}|_{max} - |\vec{R}_{BC}|_{min} = 0.1022$ Å. Thus, setting $|\vec{R}_{BC}|(i) = |\vec{R}_{BC}(e)| = 2.2816$ Å at $T_1 = 300$ K (instead of

choosing $|\vec{R}_{BC}|$ from a Maxwell-Boltzmann distribution for V_1) results in, at most, an error of one part in 44 for the extreme case of an internuclear separation corresponding to one of the classical turning points instead of to $|\vec{R}_{BC}(e)|$. Trial runs choosing between 1000 and 10 000 molecules at T_1 of 300 and 1800 K from the preceding formulas yielded initial energies that were distributed very close to the required Maxwell-Boltzmann distributions over that temperature range. This shows that for the purpose of choosing initial conditions, the approximation $|R_{BC}|(i) = |R_{BC}(e)|$ is adequate not only at $T_1 = 300$ K, but at much higher temperatures as well.

APPENDIX D

SINGLE-COLLISION PROBABILITY DISTRIBUTIONS

Probability distributions for the molecule undergoing a change $\left(\Delta H_{BC},\ \Delta\left|\vec{M}_{BC}\right|^2\right)$ per collision with an argon atom randomly selected from the heat bath are presented and updated in this appendix (tables VI and VII) in the form discussed in references 2 and 3. A family of such distributions is illustrated schematically in figure 14. (See also fig. 13). Each distribution curve depends on all the initial conditions

$$f(\Delta H_{BC}) = f\left(\Delta H_{BC};\ H_{BC}(i),\ \left|\vec{M}_{BC}\right|^2(i),\ T_2\right)$$

$$f\left(\Delta\left|\vec{M}_{BC}\right|^2\right) = f\left(\Delta\left|\vec{M}_{BC}\right|^2;\ H_{BC}(i),\ \left|\vec{M}_{BC}\right|^2(i),\ T_2\right)$$

so that each set of initial conditions $\left(H_{BC}(i),\ \left|\vec{M}_{BC}\right|^2(i),\ T_2\right)$ determines a specific distribution for ΔH_{BC} and a specific distribution for $\Delta\left|\vec{M}_{BC}\right|^2$. For an initial angular momentum $\left|\vec{M}_{BC}\right|^2(i) = 0$, the distributions $f\left(\Delta\left|\vec{M}_{BC}\right|^2\right)$ would consist of only a "gains" branch. A statistical equilibrium for ΔH_{BC} or $\Delta\left|\vec{M}_{BC}\right|^2$ would result if "gains" and "losses" branches for the corresponding distributions were symmetric, whereas a relaxation would occur if either a "gains" or a "losses" branch were predominant. The form of tabulation used in this appendix is convenient for displaying the overall relation between gains and losses branches of a given distribution but does not show the correlation between ΔH_{BC} and $\Delta\left|\vec{M}_{BC}\right|^2$ changes that is needed for an actual rate calculation. Such correlation is incorporated into the functions F_i that are given in tabular form in appendix F.

TABLE VI. - PROBABILITY DISTRIBUTIONS FOR CHANGE IN INTERNAL ENERGY OF Br_2, ΔH_{BC}, AND IN ANGULAR MOMENTUM SQUARED, $\Delta|\bar{M}_{BC}|^2$, PER COLLISION AT HEAT-BATH TEMPERATURE OF 1800 K, WITH $\left(H_{BC}(i)/H_{BC,max}\right) << 1$

[Entry n means given interval is within noise level; all entries except $H_{BC}(i) = 0.5\ D_e$, $|\bar{M}_{BC}|^2(i) = 0$ are based on 1000 real collisions (RCOL); exception contains 1756 RCOL; estimate of reliability for fractional populations is ±0.01.]

$\frac{H_{BC}(i)}{{}^{a}D_e}$	$\frac{H_{BC}(i)}{H_{BC,max}}$	$\lvert\bar{M}_{BC}\rvert^2(i)$	$\frac{\sum(RCOL^{b})}{\sum(RCOL+NCOL^{c})}$	W_1/W_2 where $W_1 = \int_X^Y f(\Delta H_{BC})d(\Delta H_{BC})$, $W_2 = \int_X^Y f\left(\Delta\lvert\bar{M}_{BC}\rvert^2\right)d\left(\Delta\lvert\bar{M}_{BC}\rvert^2\right)$, $\left(\int_{-\infty}^{+\infty} = 1\right)$										
				Integral lower limit, X										
				$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	-n	0.0001	0.001	0.01	0.1	1.0
				Integral upper limit, Y										
				-1.0	-0.1	-0.01	-0.001	-0.0001	n	∞	∞	∞	∞	∞
0	0	0	[d]0.308	0/0	0/0	0/0	0/0	0/0	0.760/0.721	0.240/n	0.189/0.279	0.062/0.233	0/0.173	0/0.042
0.1	0.100	0	0.318	0/0	0/0	0.000/0	0.005/0	0.015/0	0.758/0.713	0.227/n	0.176/0.287	0.062/0.234	0.001/0.171	0/0.046
0.1	0.100	0.01	0.315	0/0	0/0	0/0	0.008/0.040	0.028/n	0.742/0.696	0.230/n	0.177/0.264	0.060/0.231	0/0.169	0/0.044
0.1	0.100	0.1	0.315	0/0	0/0	0.001/0.060	0.024/0.076	0.078/n	0.712/0.688	0.210/n	0.167/0.235	0.062/0.217	0.000/0.162	0/0.039
0.1	0.099	1.0	0.315	0/0	0/0.096	0.026/0.137	0.108/0.144	0.139/n	0.697/0.686	0.164/n	0.139/0.170	0.061/0.162	0.000/0.130	0/0.048
0.1	0.098	2.0	0.310	0/0.046	0/0.125	0.066/0.156	0.134/0.162	0.158/n	0.699/0.691	0.143/n	0.121/0.147	0.052/0.141	0/0.111	0/0.037
0.5	0.500	0	0.336	0/0	0/0	0.011/0	0.035/0	0.052/0	0.744/0.695	0.204/n	0.160/0.305	0.058/0.240	0/0.181	0/0.058
0.5	0.500	0.01	0.344	0/0	0/0	0.015/0	0.038/0.042	0.065/n	0.720/0.669	0.214/n	0.162/0.289	0.058/0.252	0/0.186	0/0.056
0.5	0.500	0.1	0.343	0/0	0/0	0.014/0.066	0.050/0.088	0.101/n	0.692/0.661	0.207/n	0.160/0.251	0.061/0.233	0/0.173	0/0.055
0.5	0.495	1.0	0.340	0/0	0/0.099	0.032/0.138	0.111/0.145	0.151/n	0.669/0.660	0.180/n	0.145/0.195	0.068/0.189	0/0.145	0/0.059
0.5	0.493	1.48	0.342	0/0.021	0/0.120	0.034/0.166	0.132/0.174	0.171/n	0.675/0.660	0.154/n	0.120/0.166	0.047/0.155	0.000/0.116	0/0.040
0.5	0.490	2.0	0.337	0/0.048	0/0.135	0.065/0.171	0.149/0.175	0.181/n	0.671/0.664	0.148/n	0.123/0.161	0.059/0.156	0.000/0.123	0/0.050
0.5	0.476	5.0	0.328	0/0.109	0.001/0.169	0.121/0.198	0.177/0.202	0.199/n	0.680/0.673	0.121/n	0.099/0.124	0.041/0.120	0/0.095	0/0.034
0.5	0.455	10.0	0.315	0/0.118	0.006/0.175	0.131/0.200	0.180/0.205	0.201/n	0.694/0.686	0.105/n	0.087/0.109	0.042/0.103	0/0.085	0/0.032
0.9	0.900	0	0.409	0/0	0/0	0.036/0	0.093/0	0.138/0	0.655/0.617	0.208/n	0.160/0.383	0.072/0.293	0/0.214	0/0.089
0.9	0.900	0.01	0.399	0/0	0/0	0.038/0	0.095/0.055	0.150/n	0.654/0.612	0.196/n	0.145/0.332	0.061/0.286	0/0.206	0/0.088
0.9	0.899	0.1	0.397	0/0	0.000/0	0.039/0.080	0.099/0.098	0.169/n	0.625/0.609	0.205/n	0.144/0.292	0.062/0.277	0/0.203	0/0.085
0.9	0.891	1.0	0.392	0/0	0.001/0.111	0.044/0.158	0.128/0.165	0.188/n	0.617/0.610	0.195/n	0.150/0.225	0.071/0.221	0/0.173	0/0.087
0.9	0.882	2.0	0.384	0/0.051	0.001/0.131	0.066/0.172	0.145/0.177	0.187/n	0.627/0.616	0.187/n	0.152/0.206	0.069/0.202	0/0.163	0/0.081
0.9	0.857	5.0	0.368	0/0.110	0.002/0.180	0.117/0.207	0.187/0.213	0.215/n	0.643/0.632	0.142/n	0.119/0.154	0.055/0.149	0.000/0.125	0/0.063
0.9	0.818	10.0	0.340	0/0.148	0.015/0.196	0.153/0.216	0.204/0.221	0.227/n	0.670/0.661	0.103/n	0.081/0.118	0.036/0.113	0/0.088	0/0.039
0.9	0.756	19.0	0.314	0/0.140	0.031/0.196	0.147/0.218	0.192/0.223	0.212/n	0.697/0.689	0.091/n	0.077/0.088	0.032/0.084	0/0.067	0/0.028

[a]Dissociation energy for Br_2 ground state, 0.31916 u.

[b]Real collisions.

[c]Null collisions.

[d]Trajectories determined by fixed step size.

TABLE VII. - PROBABILITY DISTRIBUTIONS FOR CHANGE IN INTERNAL ENERGY OF Br_2, ΔH_{BC}, AND IN ANGULAR MOMENTUM SQUARED, $\Delta|\vec{M}_{BC}|^2$, PER COLLISION AT HEAT-BATH TEMPERATURE OF 1800 K, WITH $(H_{BC}(i)/H_{BC,max}) = 0.999$

[All entries are based on a sample size of 1519 trajectories; entry n means given interval is within noise level.]

$\frac{H_{BC}(i)}{{}^aD_e}$	$\|\vec{M}_{BC}\|^2(i)$	Fraction of sample dissociated	$\frac{\sum(\text{Dissociation events with } \|\vec{M}_{BC}\|^2 \text{ loss})}{\sum(\text{Dissociation events with } \|\vec{M}_{BC}\|^2 \text{ gain})}$	W_1/W_2 where $W_1 = \int_X^Y f(\Delta H_{BC})d(\Delta H_{BC})$, $W_2 = \int_X^Y f\left(\Delta\|\vec{M}_{BC}\|^2\right)d\left(\Delta\|\vec{M}_{BC}\|^2\right)$, $\left(\int_{-\infty}^{+\infty} = 1\right)$										
				Integral lower limit, X										
				$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	-n	0.0001	0.001	0.01	0.1	1.0
				Integral upper limit, Y										
				-1.0	-0.1	-0.01	-0.001	-0.0001	n	∞	∞	∞	∞	∞
0.999	0	0.347	0	0/0	0/0	0/0	0.007/0	0.072/0	0.419/0.354	0.508/n	0.232/0.646	0.093/0.466	0/0.288	0/0.167
1.009	1.0	0.642	0.92	0/0	0/0.151	0/0.320	0.043/0.409	0.192/n	0.346/0.055	0.463/n	0.238/0.535	0.096/0.447	0/0.313	0/0.160
1.029	3.0	0.935	1.25	0/0.067	0/0.236	0.001/0.392	0.123/0.463	0.281/n	0.309/0.041	0.410/n	0.225/0.495	0.099/0.438	0/0.306	0/0.153
1.059	6.0	0.924	1.27	0/0.101	0/0.275	0.026/0.424	0.172/0.483	0.348/n	0.270/0.033	0.382/n	0.226/0.485	0.100/0.429	0.001/0.317	0/0.157
1.099	10.0	0.868	1.09	0/0.140	0/0.304	0.065/0.446	0.190/0.506	0.369/n	0.255/0.036	0.375/n	0.233/0.458	0.087/0.405	0.001/0.293	0/0.150
1.124	12.5	0.631	0.79	0/0.155	0/0.308	0.089/0.459	0.217/0.527	0.359/n	0.280/0.033	0.361/n	0.195/0.440	0.069/0.372	0.001/0.248	0/0.118
1.149	15.0	0.058	0.63	0/0.162	0.012/0.266	0.147/0.453	0.215/0.554	0.335/n	0.484/0.051	0.181/n	0.105/0.395	0.043/0.314	0/0.158	0/0.055
1.199	20.0	0.026	0.77	0/0.156	0.021/0.230	0.151/0.399	0.201/0.557	0.294/n	0.517/0.051	0.190/n	0.088/0.392	0.041/0.267	0/0.128	0/0.043

[a]Dissociation energy for Br_2 ground state, 0.31916 u.

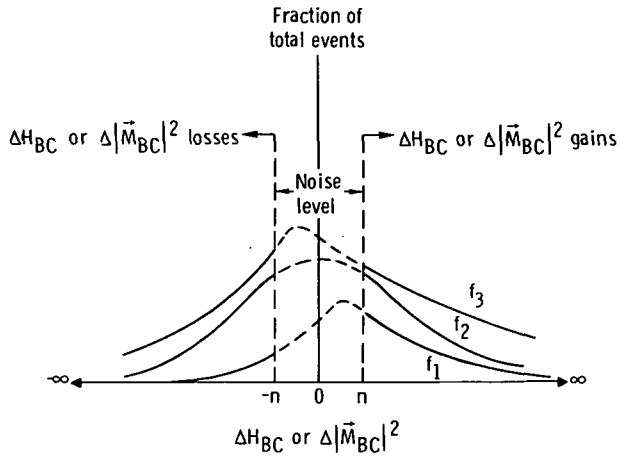


Figure 14. - Schematic drawing of a family of probability distributions, f_1, f_2, f_3, . . ., for internal energy changes ΔH_{BC} or angular momentum changes $\Delta|\vec{M}_{BC}|^2$ per collision.

APPENDIX E

TABULATIONS FOR RELAXATION OF A SAMPLE OF 10 000 MOLECULES WITH PRESHOCKED-GAS TEMPERATURE OF 300 K IN A HEAT BATH OF ARGON ATOMS AT HEAT-BATH TEMPERATURE OF 1800 K: ANGULAR MOMENTUM INCLUDED AND EXCLUDED

Three kinds of tabulations are included in this appendix. The first gives the number of molecules left undissociated after n collisions, the total system energy and angular momentum squared after n collisions (which includes both dissociated and undissociated molecules), and finally the average energy and angular momentum squared for the undissociated portion of the sample only. The second type of tabulation gives H_{BC} distributions after n collisions, and the third gives a similar distribution for $|\vec{M}_{BC}|^2$ for the case where this was included. Tabulations are given first for the case with angular momentum included, and then for the special case with $|\vec{M}_{BC}|^2 \equiv 0$.

10 000 Molecules at 300 K for 200 Collisions

NUMBER OF COLLISIONS	NUMBER OF MOLECULES LEFT UNDISSOCIATED	TOTAL ENERGY OF SYSTEM	TOTAL ANGULAR MOMENTUM SQUARED	AVERAGE ENERGY OF UNDISSOCIATED MOLECULES	AVERAGE ANGULAR MOMENTUM SQUARED
*****	*****	**********	**********	**********	**********
0	10000	63.0621743	2880.09607	0.63062174E-02	0.28800961
1	10000	81.1952009	3724.21515	0.81195200E-02	0.37242151
2	10000	96.9014101	4470.59131	0.96901410E-02	0.44705912
3	10000	111.227612	5088.67615	0.11122761E-01	0.50886761
4	10000	126.096784	5779.12152	0.12609678E-01	0.57791215
5	10000	140.638620	6404.05542	0.14063862E-01	0.64040554
6	10000	155.172915	7042.66272	0.15517291E-01	0.70426627
7	10000	167.661533	7533.65106	0.16766153E-01	0.75336510
8	10000	182.298843	8139.64136	0.18229884E-01	0.81396413
9	10000	195.984568	8710.37610	0.19598457E-01	0.87103760
10	10000	207.962692	9189.19824	0.20796259E-01	0.91891982
11	10000	220.119656	9651.79834	0.22011966E-01	0.96517983
12	10000	231.970968	10109.0333	0.23197097E-01	1.01090333
13	10000	243.095909	10540.4175	0.24309591E-01	1.05404174
14	10000	253.606056	10930.0880	0.25360605E-01	1.09300879
15	10000	262.989296	11267.3210	0.26298929E-01	1.12673210
16	9999	272.082912	11616.5591	0.27166359E-01	1.15887870
17	9999	281.902607	11916.5737	0.28148428E-01	1.18888317
18	9999	290.029758	12164.6249	0.28961223E-01	1.21369079
19	9999	299.375187	12486.1554	0.29895860E-01	1.24584703
20	9999	308.048641	12776.1823	0.30763292E-01	1.27485259
21	9999	317.585461	13082.0338	0.31717069E-01	1.30544086
22	9999	324.158581	13236.5511	0.32374447E-01	1.32089411
23	9999	331.721310	13478.4944	0.33130795E-01	1.34509088
24	9999	339.558186	13690.8129	0.33914561E-01	1.36632483
25	9999	345.979050	13856.3378	0.34556712E-01	1.38287897
26	9999	353.810764	14092.6311	0.35339962E-01	1.40651054
27	9999	361.678375	14396.9521	0.36126801E-01	1.43694578
28	9999	368.685532	14636.2716	0.36827587E-01	1.46088010
29	9999	374.037579	14710.5662	0.37362846E-01	1.46831031
30	9999	380.933880	14909.3667	0.38052544E-01	1.48819239
31	9999	386.668098	15046.8713	0.38626024E-01	1.50194423
32	9999	392.717358	15210.7323	0.39231010E-01	1.51833194
33	9999	397.970058	15267.3851	0.39756332E-01	1.52399778
34	9999	404.510887	15441.3396	0.40410480E-01	1.54139496
35	9999	410.457928	15601.1163	0.41005244E-01	1.55737424
36	9999	414.870068	15590.2283	0.41446502E-01	1.55628535
37	9998	419.136955	15676.6748	0.41842283E-01	1.56470616
38	9998	424.236340	15819.0264	0.42352324E-01	1.57894419
39	9998	430.111107	15990.3575	0.42939919E-01	1.59608068
40	9998	435.547520	16163.8677	0.43483658E-01	1.61343515
41	9998	440.736069	16332.0565	0.44002627E-01	1.63025743
42	9998	446.326641	16401.1926	0.44561795E-01	1.63717248
43	9998	452.393730	16501.7070	0.45168626E-01	1.64722598
44	9998	458.701462	16635.7161	0.45799525E-01	1.66062960
45	9998	465.767876	16842.1433	0.46506308E-01	1.68127649
46	9998	470.881428	16972.7144	0.47017765E-01	1.69433618
47	9998	474.340206	17001.2883	0.47363712E-01	1.69719410
48	9998	477.989460	17042.0632	0.47728711E-01	1.70127238
49	9998	483.111454	17213.0820	0.48241012E-01	1.71837775

NUMBER OF COLLISIONS *****	NUMBER OF MOLECULES LEFT UNDISSOCIATED *****	TOTAL ENERGY OF SYSTEM **********	TOTAL ANGULAR MOMENTUM SQUARED **********	AVERAGE ENERGY OF UNDISSOCIATED MOLECULES **********	AVERAGE ANGULAR MOMENTUM SQUARED **********
50	9998	487.724087	17316.5640	0.48702368E-01	1.72872792
51	9998	492.631237	17411.5811	0.49193181E-01	1.73823164
52	9998	496.544205	17436.4905	0.49584556E-01	1.74072304
53	9998	500.916039	17552.9521	0.50021827E-01	1.75237149
54	9998	506.359013	17705.2986	0.50566233E-01	1.76760918
55	9998	510.982769	17837.4075	0.51028701E-01	1.78082274
56	9998	513.649406	17893.8044	0.51295421E-01	1.78646351
57	9998	519.630470	18037.6230	0.51893646E-01	1.80084835
58	9997	523.468987	18153.9255	0.52248154E-01	1.81232609
59	9997	528.206039	18227.0913	0.52722002E-01	1.81964485
60	9997	531.047562	18183.2642	0.53006241E-01	1.81526087
61	9997	534.743416	18239.8110	0.53375938E-01	1.82091722
62	9997	538.999550	18257.2515	0.53801679E-01	1.82266179
63	9997	542.477776	18279.1707	0.54149606E-01	1.82485436
64	9997	545.872345	18363.5071	0.54489164E-01	1.83329046
65	9997	548.743134	18474.5693	0.54776326E-01	1.84440006
66	9997	552.024391	18481.6965	0.55104553E-01	1.84511298
67	9997	556.167458	18520.5620	0.55518984E-01	1.84900074
68	9997	561.809006	18715.8650	0.56083309E-01	1.86853692
69	9996	565.512276	18771.5115	0.56426593E-01	1.87423660
70	9996	568.524971	18742.5923	0.56727983E-01	1.87134357
71	9996	571.286255	18766.2297	0.57004221E-01	1.87370822
72	9996	575.126404	18905.6357	0.57388389E-01	1.88765436
73	9996	577.268967	18784.2124	0.57602734E-01	1.87550713
74	9996	580.709084	18829.1260	0.57946880E-01	1.88000038
75	9996	585.318909	18902.7507	0.58408049E-01	1.88736580
76	9996	587.206116	18847.5095	0.58596846E-01	1.88183942
77	9996	589.771538	18875.0269	0.58853490E-01	1.88459231
78	9996	594.110207	18885.3940	0.59287529E-01	1.88562952
79	9995	599.415215	18967.3066	0.59790303E-01	1.89369623
80	9995	601.215736	19057.4583	0.59970445E-01	1.90271591
81	9995	604.566132	19109.6233	0.60305650E-01	1.90793492
82	9995	609.324203	19302.2559	0.60781698E-01	1.92720786
83	9995	613.151268	19404.0132	0.61164597E-01	1.93738863
84	9994	616.082664	19444.6309	0.61431576E-01	1.94148478
85	9994	619.873085	19522.4871	0.61810841E-01	1.94927520
86	9993	622.638077	19524.0774	0.62040693E-01	1.94943073
87	9993	623.034660	19410.3120	0.62080380E-01	1.93804625
88	9993	624.417198	19393.3281	0.62218732E-01	1.93634659
89	9992	626.524750	19437.8677	0.62400972E-01	1.94050047
90	9992	629.985046	19571.2361	0.62747279E-01	1.95384799
91	9992	632.026985	19531.0061	0.62951637E-01	1.94982170
92	9991	635.264473	19675.0247	0.63217368E-01	1.96426356
93	9991	637.859657	19702.4270	0.63477120E-01	1.96700627
94	9991	640.494797	19754.3535	0.63740871E-01	1.97220357
95	9991	643.819305	19820.8801	0.64073621E-01	1.97886232
96	9991	644.369576	19904.9941	0.64128696E-01	1.98728117
97	9991	646.344467	19926.9407	0.64326365E-01	1.98947793
98	9991	648.286705	20013.9463	0.64520764E-01	1.99818623
99	9991	650.693916	20045.3899	0.64761702E-01	2.00133348

NUMBER OF COLLISIONS *****	NUMBER OF MOLECULES LEFT UNDISSOCIATED *****	TOTAL ENERGY OF SYSTEM **********	TOTAL ANGULAR MOMENTUM SQUARED **********	AVERAGE ENERGY OF UNDISSOCIATED MOLECULES **********	AVERAGE ANGULAR MOMENTUM SQUARED **********
100	9991	652.274658	20092.0488	0.64919917E-01	2.00600353
101	9991	657.173615	20263.0850	0.65410254E-01	2.02312255
102	9991	658.333977	20172.9004	0.65526394E-01	2.01409596
103	9990	661.619194	20290.4963	0.65828216E-01	2.02584070
104	9990	661.893112	20278.0566	0.65855638E-01	2.02459550
105	9990	662.066048	20178.4431	0.65872946E-01	2.01462421
106	9990	664.529465	20245.0193	0.66119536E-01	2.02128848
107	9990	666.288734	20272.3147	0.66295639E-01	2.02402079
108	9990	667.955086	20208.9790	0.66462440E-01	2.01768085
109	9989	669.802406	20242.2649	0.66590645E-01	2.02093312
110	9989	672.648468	20349.3528	0.66875567E-01	2.03165351
111	9989	674.313553	20423.3584	0.67042260E-01	2.03906247
112	9989	676.055626	20448.7378	0.67216657E-01	2.04160315
113	9989	677.037064	20463.2483	0.67314911E-01	2.04305577
114	9988	679.491867	20560.5815	0.67524320E-01	2.05151686
115	9988	681.639572	20552.8115	0.67739346E-01	2.05073887
116	9986	682.823517	20539.0371	0.67804252E-01	2.04894638
117	9986	684.412445	20540.3843	0.67963368E-01	2.04908127
118	9986	686.679497	20606.5645	0.68190391E-01	2.05570856
119	9985	689.637070	20654.3354	0.68460666E-01	2.06058279
120	9985	690.367622	20552.2922	0.68533829E-01	2.05036315
121	9985	693.262169	20639.0774	0.68823717E-01	2.05905476
122	9984	693.856880	20653.6794	0.68849312E-01	2.05871907
123	9984	693.433380	20545.4534	0.68806895E-01	2.04787910
124	9984	695.069283	20597.0889	0.68970748E-01	2.05305085
125	9984	697.335487	20597.5559	0.69197726E-01	2.05309761
126	9983	699.014221	20612.2871	0.69337315E-01	2.05396217
127	9983	699.944046	20608.8516	0.69430455E-01	2.05361801
128	9982	701.055023	20577.1665	0.69516714E-01	2.05064788
129	9981	703.478180	20631.4048	0.69729456E-01	2.05616024
130	9979	704.560020	20770.4006	0.69777921E-01	2.06889421
131	9979	706.976257	20792.0613	0.70020056E-01	2.07106477
132	9979	708.566429	20843.1104	0.70179407E-01	2.07618049
133	9979	707.043686	20689.7163	0.70026812E-01	2.06080875
134	9979	708.654457	20741.8140	0.70188227E-01	2.06602943
135	9979	708.885765	20735.8760	0.70211407E-01	2.06543446
136	9979	709.418945	20750.5190	0.70264836E-01	2.06690189
137	9977	711.051208	20797.3525	0.70373259E-01	2.07146716
138	9977	713.005066	20880.8088	0.70569122E-01	2.07983202
139	9976	714.242027	20860.5393	0.70663385E-01	2.07783461
140	9976	714.964279	20891.8296	0.70735781E-01	2.08014110
141	9976	716.800682	20890.4475	0.70919863E-01	2.08000249
142	9976	716.370110	20832.9495	0.70876702E-01	2.07423902
143	9975	717.357582	20743.3328	0.70947449E-01	2.06443033
144	9975	719.883392	20807.8162	0.71200661E-01	2.07089454
145	9974	720.946693	20847.9407	0.71249190E-01	2.07503381
146	9974	721.241692	20875.1423	0.71278768E-01	2.07776099
147	9974	723.036964	20929.9978	0.71458763E-01	2.08326080
148	9974	723.677505	20891.9810	0.71522984E-01	2.07944930
149	9973	725.354195	21001.7690	0.71612891E-01	2.09051943

NUMBER OF COLLISIONS *****	NUMBER OF MOLECULES LEFT UNDISSOCIATED *****	TOTAL ENERGY OF SYSTEM **********	TOTAL ANGULAR MOMENTUM SQUARED **********	AVERAGE ENERGY OF UNDISSOCIATED MOLECULES **********	AVERAGE ANGULAR MOMENTUM SQUARED **********
150	9973	724.398239	20907.5015	0.71517037E-01	2.08106712
151	9972	726.529137	20942.0054	0.71703266E-01	2.08434030
152	9972	727.602959	21014.2505	0.71810952E-01	2.09158516
153	9972	728.325745	21024.6501	0.71883436E-01	2.09262830
154	9971	729.894234	21017.2090	0.72012207E-01	2.09178615
155	9970	730.880035	21001.8774	0.72080091E-01	2.08870852
156	9968	730.141457	20890.7910	0.71953927E-01	2.07743478
157	9968	730.959366	20776.4297	0.72035982E-01	2.06596193
158	9968	730.017906	20761.5911	0.71941537E-01	2.06447318
159	9967	731.783653	20868.9343	0.72091955E-01	2.07501081
160	9967	733.331245	20836.7534	0.72247226E-01	2.07178217
161	9967	734.395905	20904.4971	0.72354048E-01	2.07857904
162	9967	736.469269	20900.3408	0.72562065E-01	2.07816195
163	9967	738.364601	20972.9153	0.72752229E-01	2.08544344
164	9967	740.290199	20964.9905	0.72945426E-01	2.08464828
165	9967	739.680244	20971.8594	0.72884228E-01	2.08533752
166	9967	740.454239	20927.9631	0.72961881E-01	2.08093327
167	9966	740.660133	20835.8167	0.72952647E-01	2.07031482
168	9966	741.501648	20865.7510	0.73037085E-01	2.07331842
169	9965	743.654762	20911.2383	0.73222145E-01	2.07624662
170	9965	744.146446	20872.4189	0.73271489E-01	2.07235110
171	9965	745.817848	20953.8213	0.73439217E-01	2.08051991
172	9965	748.534065	21030.4360	0.73711794E-01	2.08820829
173	9965	750.591438	21119.8433	0.73918255E-01	2.09718049
174	9965	751.581718	21088.2388	0.74017627E-01	2.09400895
175	9965	754.269333	21123.5815	0.74287330E-01	2.09755567
176	9963	755.224396	21185.2214	0.74326621E-01	2.10322019
177	9963	757.224953	21241.5955	0.74527421E-01	2.10887858
178	9963	759.226379	21318.6221	0.74728307E-01	2.11660990
179	9963	760.252457	21295.9377	0.74831295E-01	2.11433300
180	9961	761.625755	21335.6829	0.74906185E-01	2.11443928
181	9960	764.279709	21528.3950	0.75146472E-01	2.13365391
182	9960	764.844551	21474.9700	0.75203182E-01	2.12828985
183	9960	765.665367	21443.0137	0.75285590E-01	2.12508139
184	9960	766.391205	21415.0872	0.75358465E-01	2.12227750
185	9959	768.527245	21384.4226	0.75547379E-01	2.11922956
186	9957	770.468636	21398.5435	0.75678793E-01	2.11816186
187	9957	769.931702	21321.0056	0.75624869E-01	2.11037454
188	9956	771.581795	21302.4688	0.75760968E-01	2.10753855
189	9955	772.590614	21273.7354	0.75837016E-01	2.10469767
190	9954	773.366814	21270.5259	0.75886791E-01	2.10408589
191	9954	773.685844	21243.9404	0.75918836E-01	2.10141507
192	9953	776.805885	21333.4717	0.76202338E-01	2.11052790
193	9952	777.316956	21332.1682	0.76226708E-01	2.11006823
194	9952	775.317719	21148.8428	0.76025819E-01	2.09164709
195	9952	777.225975	21307.1140	0.76217563E-01	2.10755074
196	9952	777.723679	21256.4602	0.76267573E-01	2.10246083
197	9951	778.461662	21248.8718	0.76312954E-01	2.10053900
198	9950	777.434776	21174.1948	0.76170539E-01	2.09317309
199	9950	779.644150	21200.5554	0.76392588E-01	2.09582227

NUMBER OF COLLISIONS *****	NUMBER OF MOLECULES LEFT UNDISSOCIATED *****	TOTAL ENERGY OF SYSTEM **********	TOTAL ANGULAR MOMENTUM SQUARED **********	AVERAGE ENERGY OF UNDISSOCIATED MOLECULES **********	AVERAGE ANGULAR MOMENTUM SQUARED **********
200	9950	781.563080	21253.3672	0.76585450E-01	2.10113004

ENERGY DISTRIBUTIONS

NUMBER OF COLLISIONS	NUMBER OF UNDISSOCIATED MOLECULES WITH ENERGIES GREATER THAN -															
	.00	.01	.02	.03	.04	.05	.06	.07	.08	.09	.10	.11	.12	.13	.14	.15	.16
*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
0	10000	1865	217	23	1	1	0	0	0	0	0	0	0	0	0	0	0
1	10000	2651	704	258	116	66	30	12	2	2	2	2	1	1	1	1	1
2	10000	3260	1133	485	231	120	59	26	7	6	6	5	2	1	1	1	1
3	10000	3758	1494	687	347	197	91	44	21	12	10	7	5	3	2	2	2
4	10000	4285	1865	909	474	271	128	68	34	17	14	11	7	5	3	3	3
5	10000	4772	2239	1141	625	339	171	95	55	31	20	15	8	6	3	3	3
6	10000	5176	2619	1386	767	416	235	140	77	46	29	20	13	11	6	5	4
7	10000	5542	2907	1586	916	497	284	169	97	54	33	22	16	14	8	6	4
8	10000	5863	3235	1839	1078	614	358	224	135	86	56	38	27	15	8	7	6
9	10000	6190	3555	2059	1233	720	433	276	167	108	74	45	30	18	12	8	7
10	10000	6451	3778	2263	1383	828	499	326	199	127	90	54	38	23	15	11	10
11	10000	6685	4001	2484	1558	942	582	395	253	158	104	59	42	27	19	11	10
12	10000	6878	4230	2713	1720	1062	675	451	289	180	120	69	44	29	22	14	9
13	10000	7047	4479	2906	1856	1167	745	496	320	206	139	82	53	35	25	15	11
14	10000	7205	4650	3070	1984	1272	818	547	365	245	161	91	62	43	30	19	13
15	10000	7330	4847	3237	2095	1355	877	597	405	268	179	99	67	48	34	19	15
16	9999	7466	5002	3384	2232	1449	949	651	442	310	198	111	73	44	32	19	14
17	9999	7566	5195	3527	2358	1566	1026	700	488	333	211	117	81	53	36	25	18
18	9999	7666	5344	3632	2452	1679	1108	757	535	360	234	124	87	58	41	26	18
19	9999	7789	5527	3768	2586	1764	1184	802	572	385	255	151	110	75	44	28	20
20	9999	7895	5676	3911	2709	1874	1269	859	602	401	260	165	116	79	53	31	21
21	9999	7996	5817	4092	2824	1984	1349	935	652	445	283	181	122	87	57	33	23
22	9999	8056	5899	4198	2916	2059	1415	981	684	471	291	189	128	93	63	40	33
23	9999	8112	6023	4325	3023	2147	1478	1025	721	485	319	219	146	106	71	48	35
24	9999	8190	6108	4447	3130	2233	1545	1080	764	518	343	228	155	114	79	56	39
25	9999	8254	6226	4538	3226	2311	1605	1114	777	537	363	246	163	119	79	58	40
26	9999	8307	6333	4616	3327	2397	1677	1185	852	580	390	263	176	123	83	63	40
27	9999	8370	6439	4712	3449	2489	1751	1255	895	616	416	285	191	131	95	64	43
28	9999	8416	6526	4835	3542	2549	1827	1312	917	633	446	300	201	144	100	70	48
29	9999	8461	6592	4900	3618	2586	1884	1371	957	661	463	315	212	155	107	69	50
30	9999	8525	6669	4992	3702	2667	1951	1437	991	700	500	339	226	165	110	67	47
31	9999	8554	6753	5088	3763	2727	2019	1468	1022	731	521	354	241	177	116	69	48
32	9999	8585	6794	5168	3864	2815	2085	1483	1055	770	542	376	259	191	137	85	54
33	9999	8603	6863	5237	3923	2884	2115	1535	1085	799	556	390	266	197	147	89	60
34	9999	8637	6920	5314	4016	2976	2192	1605	1121	829	581	411	286	206	145	86	58
35	9999	8680	6977	5367	4094	3034	2246	1652	1178	860	608	432	307	213	149	97	65
36	9999	8727	7029	5434	4137	3095	2281	1668	1209	878	615	446	323	224	155	98	67
37	9998	8755	7104	5493	4205	3139	2327	1723	1235	891	619	454	327	225	152	102	67
38	9998	8778	7156	5573	4263	3228	2390	1763	1279	916	635	457	325	223	161	105	72
39	9998	8834	7212	5653	4298	3272	2429	1799	1329	970	667	476	336	236	173	116	77
40	9998	8848	7241	5706	4386	3353	2469	1845	1365	997	698	506	355	245	173	118	79
41	9998	8870	7297	5763	4452	3394	2525	1887	1418	1044	726	517	367	266	180	119	75
42	9998	8897	7334	5852	4529	3443	2579	1929	1452	1067	757	543	393	281	193	130	87
43	9998	8894	7388	5897	4608	3525	2661	2004	1486	1101	796	568	417	292	203	140	97
44	9998	8947	7446	5966	4698	3608	2730	2054	1526	1128	831	586	430	301	204	144	103
45	9998	8955	7481	6010	4773	3697	2806	2117	1597	1189	884	609	451	317	220	151	108
46	9998	8968	7529	6067	4809	3756	2873	2170	1627	1210	903	640	467	335	235	162	110
47	9998	9000	7579	6123	4864	3786	2888	2177	1644	1228	894	646	482	348	246	166	114
48	9998	9017	7629	6176	4923	3817	2888	2173	1670	1244	900	669	505	361	265	177	123
49	9998	9029	7695	6257	4970	3882	2949	2207	1697	1254	931	700	520	374	269	186	118

ENERGY DISTRIBUTIONS

NUMBER OF COLLISIONS	NUMBER OF UNDISSOCIATED MOLECULES WITH ENERGIES GREATER THAN -																
*****	.00 *****	.01 *****	.02 *****	.03 *****	.04 *****	.05 *****	.06 *****	.07 *****	.08 *****	.09 *****	.10 *****	.11 *****	.12 *****	.13 *****	.14 *****	.15 *****	.16 *****
50	9998	9045	7745	6296	4997	3930	3010	2279	1744	1291	964	720	533	380	274	187	122
51	9998	9070	7772	6344	5035	3945	3065	2338	1790	1334	1002	756	560	391	281	194	129
52	9998	9052	7795	6397	5098	3986	3095	2380	1829	1376	1020	767	567	403	294	204	138
53	9998	9096	7828	6447	5138	4035	3127	2420	1852	1399	1049	784	579	421	308	205	139
54	9998	9120	7854	6486	5196	4091	3169	2480	1899	1437	1083	818	598	435	328	216	146
55	9998	9134	7889	6532	5223	4137	3233	2533	1940	1464	1107	829	615	445	332	227	158
56	9998	9120	7906	6568	5276	4168	3260	2551	1945	1461	1120	850	628	455	334	237	166
57	9998	9132	7943	6623	5316	4220	3340	2619	1980	1521	1160	874	645	472	341	244	173
58	9997	9146	7986	6653	5372	4276	3395	2647	2001	1554	1184	876	644	483	344	243	168
59	9997	9148	8013	6718	5431	4324	3413	2675	2035	1588	1212	908	668	493	364	253	173
60	9997	9172	8010	6720	5431	4338	3431	2697	2068	1618	1227	923	693	514	370	258	179
61	9997	9187	8060	6749	5434	4375	3443	2738	2084	1632	1250	937	705	534	388	276	186
62	9997	9188	8091	6754	5495	4427	3484	2780	2126	1641	1242	946	731	537	391	296	205
63	9997	9200	8095	6789	5527	4475	3543	2835	2167	1669	1266	969	734	545	391	295	208
64	9997	9226	8104	6823	5557	4516	3576	2849	2204	1693	1272	972	757	560	401	296	207
65	9997	9238	8108	6826	5603	4545	3612	2878	2244	1721	1298	985	764	565	401	289	209
66	9997	9213	8092	6837	5625	4586	3652	2920	2295	1748	1329	1010	773	566	409	302	211
67	9997	9229	8123	6874	5656	4625	3689	2961	2331	1788	1361	1037	785	573	427	308	216
68	9997	9239	8156	6935	5724	4665	3753	3005	2383	1845	1392	1069	804	597	452	327	229
69	9996	9242	8144	6943	5757	4713	3810	3047	2415	1875	1432	1086	819	606	453	325	231
70	9996	9252	8160	6961	5771	4740	3858	3096	2448	1880	1438	1099	826	608	455	321	232
71	9996	9263	8172	6966	5819	4781	3884	3123	2457	1912	1482	1121	833	611	457	336	238
72	9996	9259	8199	7014	5836	4774	3899	3135	2460	1919	1503	1152	893	641	482	358	245
73	9996	9252	8197	7036	5868	4816	3953	3162	2473	1918	1501	1141	894	650	493	362	252
74	9996	9279	8248	7081	5910	4868	3930	3177	2490	1928	1519	1167	892	659	498	361	259
75	9996	9275	8229	7103	5929	4917	3998	3241	2569	1994	1557	1183	899	677	515	366	264
76	9996	9271	8264	7124	5962	4954	4021	3246	2585	2001	1564	1189	903	681	522	380	278
77	9996	9294	8256	7134	6003	5007	4063	3278	2589	2033	1570	1183	910	692	533	392	284
78	9996	9298	8280	7153	6033	5058	4111	3321	2606	2037	1590	1219	929	708	544	409	292
79	9995	9283	8305	7167	6065	5106	4179	3378	2667	2077	1623	1247	966	729	553	418	301
80	9995	9275	8320	7191	6088	5106	4207	3409	2687	2113	1625	1261	965	731	553	414	293
81	9995	9290	8332	7218	6102	5115	4224	3439	2722	2139	1653	1282	978	732	559	436	309
82	9995	9317	8368	7271	6126	5144	4257	3459	2774	2201	1696	1289	994	762	578	439	312
83	9995	9318	8382	7323	6192	5190	4296	3486	2788	2234	1717	1313	997	776	589	439	312
84	9994	9340	8415	7366	6235	5232	4322	3482	2798	2226	1734	1321	995	781	592	439	325
85	9994	9365	8434	7390	6258	5267	4358	3524	2825	2261	1744	1348	1004	779	605	446	325
86	9993	9365	8415	7389	6300	5284	4359	3536	2858	2289	1768	1354	1009	797	614	455	332
87	9993	9365	8407	7417	6316	5301	4333	3538	2851	2285	1781	1352	1010	797	612	462	336
88	9993	9369	8426	7415	6295	5305	4336	3547	2872	2302	1779	1369	1021	807	619	472	350
89	9992	9378	8458	7415	6320	5306	4356	3557	2863	2305	1790	1386	1053	821	630	482	360
90	9992	9400	8478	7456	6387	5330	4386	3569	2879	2316	1786	1394	1087	837	628	478	366
91	9992	9373	8472	7449	6392	5344	4394	3589	2918	2331	1809	1412	1103	858	641	477	357
92	9991	9382	8473	7473	6438	5337	4405	3631	2951	2347	1846	1431	1118	869	659	488	363
93	9991	9378	8494	7493	6445	5383	4447	3671	2982	2349	1843	1442	1122	873	651	498	368
94	9991	9393	8495	7517	6467	5432	4503	3687	2981	2378	1864	1466	1131	878	656	497	366
95	9991	9393	8492	7530	6466	5455	4536	3690	2988	2428	1905	1485	1160	894	681	510	377
96	9991	9379	8503	7559	6481	5492	4542	3710	3007	2428	1893	1464	1152	894	673	501	375
97	9991	9378	8525	7569	6502	5515	4547	3722	3004	2427	1909	1479	1165	910	677	505	378
98	9991	9391	8527	7584	6534	5515	4566	3733	3030	2440	1912	1487	1179	909	673	515	393
99	9991	9417	8564	7593	6528	5542	4582	3760	3060	2472	1921	1497	1187	912	687	516	397

ENERGY DISTRIBUTIONS

NUMBER OF COLLISIONS	NUMBER OF UNDISSOCIATED MOLECULES WITH ENERGIES GREATER THAN -															
*****	.00 *****	.01 *****	.02 *****	.03 *****	.04 *****	.05 *****	.06 *****	.07 *****	.08 *****	.09 *****	.10 *****	.11 *****	.12 *****	.13 *****	.14 *****	.15 *****	.16 *****
100	9951	9430	8596	7623	6549	5568	4612	3767	3087	2461	1923	1491	1177	899	685	522	393
101	9951	9451	8632	7643	6578	5596	4639	3804	3115	2498	1975	1532	1202	921	693	541	410
102	9951	9471	8647	7639	6551	5570	4634	3813	3110	2507	1993	1562	1214	931	697	545	423
103	9950	9480	8665	7681	6612	5603	4639	3824	3138	2528	2001	1575	1222	944	709	550	424
104	9950	9483	8645	7672	6602	5584	4662	3825	3123	2529	1992	1572	1229	957	729	568	427
105	9950	9477	8650	7665	6611	5587	4665	3823	3116	2524	2016	1589	1232	954	726	561	422
106	9950	9462	8641	7654	6623	5603	4680	3846	3159	2534	2044	1611	1263	975	741	557	423
107	9950	9450	8650	7669	6628	5647	4685	3853	3149	2533	2050	1608	1280	984	751	564	425
108	9950	9445	8626	7667	6653	5668	4688	3856	3153	2553	2071	1625	1285	1005	754	582	441
109	9949	9453	8645	7680	6658	5682	4731	3888	3173	2539	2071	1645	1299	1003	757	597	449
110	9949	9446	8636	7688	6654	5698	4767	3944	3215	2569	2093	1660	1309	1014	768	613	453
111	9949	9437	8630	7680	6668	5726	4777	3960	3220	2589	2104	1663	1323	1036	770	599	442
112	9949	9440	8642	7693	6700	5718	4795	3966	3238	2592	2112	1674	1333	1035	774	600	454
113	9949	9440	8620	7677	6669	5706	4777	3990	3276	2649	2143	1679	1343	1042	782	607	448
114	9948	9450	8628	7696	6693	5728	4825	4022	3289	2670	2161	1697	1358	1051	790	613	458
115	9948	9448	8634	7691	6698	5721	4837	4069	3331	2683	2188	1721	1361	1048	799	618	466
116	9946	9449	8617	7685	6690	5745	4859	4094	3340	2704	2175	1722	1362	1059	799	613	469
117	9946	9451	8626	7678	6708	5761	4869	4096	3352	2722	2199	1725	1371	1060	795	619	477
118	9946	9465	8642	7702	6740	5785	4886	4098	3360	2730	2205	1740	1375	1058	812	620	482
119	9945	9462	8648	7724	6751	5797	4927	4113	3383	2754	2219	1764	1399	1086	837	641	489
120	9945	9475	8673	7743	6736	5790	4948	4120	3387	2740	2228	1773	1399	1098	845	641	483
121	9945	9506	8677	7763	6773	5811	4933	4126	3409	2769	2250	1786	1414	1117	860	653	481
122	9944	9488	8670	7781	6787	5814	4932	4136	3393	2776	2261	1775	1408	1109	854	650	480
123	9944	9495	8663	7778	6770	5801	4926	4135	3394	2774	2252	1749	1399	1112	857	651	482
124	9944	9491	8645	7746	6765	5810	4943	4154	3436	2811	2276	1777	1397	1118	870	646	482
125	9944	9477	8644	7749	6758	5811	4968	4188	3463	2849	2284	1788	1405	1122	881	659	495
126	9943	9479	8667	7749	6767	5830	4983	4209	3477	2835	2262	1786	1422	1130	886	661	506
127	9943	9496	8686	7758	6777	5869	5004	4194	3465	2818	2268	1801	1421	1120	904	671	506
128	9942	9500	8680	7754	6797	5873	5015	4201	3467	2813	2290	1801	1431	1118	878	676	519
129	9941	9491	8679	7773	6814	5870	5024	4224	3480	2835	2308	1817	1451	1134	892	685	532
130	9939	9484	8675	7789	6814	5894	5045	4235	3481	2837	2313	1835	1456	1145	892	687	533
131	9939	9476	8689	7790	6827	5918	5052	4263	3501	2854	2324	1870	1481	1158	900	710	540
132	9939	9485	8701	7815	6831	5927	5065	4262	3508	2864	2327	1879	1473	1166	914	721	554
133	9939	9477	8704	7806	6824	5904	5053	4253	3483	2848	2304	1850	1454	1158	909	713	562
134	9939	9462	8710	7819	6856	5919	5054	4276	3522	2882	2328	1859	1455	1150	908	706	556
135	9939	9460	8705	7815	6843	5925	5047	4268	3534	2879	2323	1868	1468	1158	913	708	550
136	9939	9461	8711	7807	6861	5945	5063	4270	3542	2890	2333	1869	1474	1145	916	697	536
137	9937	9462	8716	7811	6850	5953	5082	4286	3537	2888	2334	1877	1485	1157	917	705	547
138	9937	9485	8723	7828	6872	5948	5072	4281	3555	2891	2357	1897	1514	1200	932	706	550
139	9936	9474	8745	7794	6833	5953	5069	4295	3577	2928	2378	1930	1538	1204	941	718	557
140	9936	9467	8731	7801	6842	5947	5064	4282	3561	2944	2381	1938	1544	1227	954	737	562
141	9936	9488	8726	7806	6861	5942	5088	4303	3599	2972	2418	1963	1552	1232	964	738	559
142	9936	9465	8733	7810	6854	5944	5082	4276	3593	2952	2412	1974	1559	1248	966	737	550
143	9935	9473	8711	7823	6881	5975	5101	4314	3624	2948	2419	1966	1558	1237	964	738	559
144	9935	9484	8724	7839	6890	5963	5107	4311	3629	2984	2438	1983	1573	1250	955	734	562
145	9934	9479	8722	7858	6933	5978	5098	4290	3617	2992	2434	2003	1588	1226	960	739	564
146	9934	9473	8745	7855	6910	5967	5089	4292	3629	2991	2436	2002	1593	1239	966	738	562
147	9934	9478	8733	7831	6920	5974	5102	4313	3647	3023	2453	2020	1606	1252	971	746	567
148	9934	9477	8736	7844	6912	5989	5122	4340	3639	3012	2447	1996	1589	1255	972	752	573
149	9933	9464	8746	7843	6914	5991	5142	4339	3651	3013	2457	2019	1601	1272	979	757	574

ENERGY DISTRIBUTIONS

NUMBER OF COLLISIONS	NUMBER OF UNDISSOCIATED MOLECULES WITH ENERGIES GREATER THAN -																
*****	.00	.01	.02	.03	.04	.05	.06	.07	.08	.09	.10	.11	.12	.13	.14	.15	.16
150	9973	9472	8744	7837	6919	6007	5124	4344	3643	2992	2438	1988	1582	1250	973	755	569
151	9972	9480	8751	7853	6925	6019	5143	4356	3637	2985	2446	1988	1593	1275	989	769	581
152	9972	9486	8761	7855	6935	6042	5143	4353	3637	2984	2443	1977	1581	1254	991	775	592
153	9972	9499	8728	7828	6938	6053	5182	4358	3662	3002	2455	1981	1597	1257	1006	771	579
154	9971	9494	8740	7832	6938	6059	5186	4389	3647	3001	2472	2004	1603	1271	1014	785	593
155	9970	9486	8745	7841	6962	6080	5191	4402	3653	2994	2459	1991	1593	1277	1030	800	610
156	9968	9475	8734	7827	6952	6055	5203	4391	3675	2985	2464	2001	1589	1271	1007	773	592
157	9968	9434	8732	7834	6939	6075	5179	4377	3688	3018	2479	2018	1628	1291	1026	771	588
158	9968	9437	8727	7825	6928	6062	5186	4365	3672	3035	2489	2029	1624	1297	1017	769	586
159	9967	9445	8722	7830	6924	6074	5207	4411	3696	3042	2500	2048	1622	1308	1027	771	594
160	9967	9427	8709	7809	6907	6039	5211	4443	3736	3074	2515	2084	1665	1308	1028	766	591
161	9967	9431	8694	7826	6890	6030	5206	4451	3751	3083	2534	2079	1674	1310	1037	779	597
162	9967	9439	8699	7844	6922	6042	5209	4461	3755	3098	2544	2078	1658	1321	1052	802	605
163	9967	9459	8706	7841	6926	6061	5217	4470	3781	3138	2563	2100	1659	1314	1046	807	608
164	9967	9471	8740	7869	6952	6085	5230	4481	3785	3135	2566	2113	1671	1320	1047	813	612
165	9967	9474	8757	7869	6967	6111	5243	4479	3773	3122	2579	2090	1653	1310	1039	811	615
166	9967	9488	8760	7864	6958	6096	5255	4484	3761	3119	2589	2102	1670	1321	1043	814	622
167	9966	9494	8792	7871	6981	6075	5239	4474	3741	3110	2591	2092	1670	1302	1019	813	625
168	9966	9494	8812	7905	6998	6091	5245	4480	3761	3105	2573	2082	1666	1287	1021	813	630
169	9965	9495	8808	7888	6958	6082	5259	4497	3764	3123	2589	2121	1684	1310	1045	833	637
170	9965	9482	8802	7902	6966	6109	5273	4507	3788	3129	2573	2100	1672	1318	1053	818	634
171	9965	9488	8798	7898	6967	6124	5302	4516	3796	3154	2583	2104	1677	1334	1056	816	640
172	9965	9471	8804	7916	6990	6126	5324	4554	3840	3173	2602	2108	1688	1348	1073	836	661
173	9965	9486	8820	7924	6998	6134	5342	4555	3854	3206	2608	2112	1692	1362	1084	847	662
174	9965	9494	8819	7917	7002	6140	5360	4555	3827	3194	2611	2115	1712	1379	1087	851	663
175	9965	9503	8815	7951	7034	6164	5376	4550	3853	3202	2636	2142	1717	1386	1102	852	671
176	9963	9508	8829	7977	7038	6168	5372	4579	3849	3222	2636	2137	1722	1375	1090	842	648
177	9963	9506	8837	7998	7065	6197	5392	4610	3858	3235	2631	2148	1724	1381	1091	839	653
178	9963	9519	8853	7993	7087	6233	5410	4628	3866	3227	2654	2150	1722	1384	1093	848	663
179	9963	9518	8863	8003	7096	6240	5391	4641	3877	3228	2656	2158	1726	1393	1090	854	681
180	9961	9518	8840	7991	7099	6272	5425	4650	3898	3227	2659	2181	1745	1394	1088	862	674
181	9960	9516	8839	8001	7097	6274	5441	4681	3920	3255	2681	2183	1755	1395	1104	877	693
182	9960	9535	8852	7984	7080	6271	5441	4665	3925	3254	2689	2203	1759	1401	1116	881	687
183	9960	9542	8857	7977	7092	6268	5434	4674	3927	3268	2713	2216	1762	1399	1124	889	697
184	9960	9531	8876	8003	7128	6289	5423	4645	3903	3268	2724	2235	1761	1389	1118	878	691
185	9959	9528	8863	8022	7125	6298	5443	4668	3908	3286	2751	2279	1795	1387	1127	886	687
186	9957	9532	8861	8023	7141	6297	5430	4688	3933	3283	2745	2280	1815	1425	1139	874	692
187	9957	9544	8841	8006	7132	6303	5460	4680	3923	3267	2734	2259	1823	1401	1130	875	691
188	9956	9554	8853	8024	7146	6312	5461	4671	3903	3256	2713	2249	1838	1408	1138	896	707
189	9955	9547	8866	8030	7176	6323	5473	4675	3920	3270	2721	2241	1825	1415	1137	894	713
190	9954	9532	8854	8018	7191	6336	5489	4704	3938	3289	2733	2231	1805	1429	1141	895	707
191	9954	9533	8850	8041	7198	6334	5495	4694	3928	3279	2728	2234	1797	1423	1134	890	709
192	9953	9515	8824	8023	7188	6355	5503	4715	3942	3305	2745	2267	1830	1461	1174	919	738
193	9952	9495	8804	8000	7189	6353	5522	4735	3956	3308	2748	2259	1819	1457	1181	917	740
194	9952	9517	8792	7943	7148	6302	5485	4705	3949	3311	2757	2269	1830	1475	1196	931	733
195	9952	9526	8806	7976	7144	6286	5469	4728	3950	3347	2784	2294	1858	1487	1202	937	742
196	9952	9533	8818	7976	7175	6291	5489	4745	3971	3342	2772	2283	1850	1490	1212	958	747
197	9951	9542	8852	8010	7141	6273	5485	4723	3955	3328	2776	2288	1857	1510	1228	968	752
198	9950	9532	8820	8002	7144	6245	5487	4691	3925	3309	2778	2251	1831	1512	1237	979	752
199	9950	9548	8832	8001	7150	6270	5498	4703	3937	3310	2784	2255	1842	1509	1245	978	764

ENERGY DISTRIBUTIONS

NUMBER OF COLLISIONS	NUMBER OF UNDISSOCIATED MOLECULES WITH ENERGIES GREATER THAN -																	
	.00	.01	.02	.03	.04	.05	.06	.07	.08	.09	.10	.11	.12	.13	.14	.15	.16
*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
200	9950	9545	8851	8018	7165	6288	5513	4720	3946	3319	2786	2265	1869	1517	1241	975	766

ENERGY DISTRIBUTIONS

NUMBER OF COLLISIONS	NUMBER OF UNDISSOCIATED MOLECULES WITH ENERGIES GREATER THAN -																
*****	.17 *****	.18 *****	.19 *****	.20 *****	.21 *****	.22 *****	.23 *****	.24 *****	.25 *****	.26 *****	.27 *****	.28 *****	.29 *****	.30 *****	.31 *****	.32 *****	*****
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
2	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
3	2	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	
4	3	1	1	1	1	1	1	1	1	1	1	1	1	1	0	0	
5	2	1	1	1	1	1	1	1	1	1	1	1	1	1	0	0	
6	3	1	1	1	1	1	1	1	1	1	1	1	1	1	1	0	
7	3	2	2	2	2	1	1	1	1	1	1	1	1	1	1	1	
8	5	2	2	2	2	1	1	1	1	1	1	1	1	1	1	1	
9	6	2	2	2	2	1	1	1	1	1	1	1	1	1	1	1	
10	8	3	3	3	1	1	1	1	1	1	1	1	1	1	1	1	
11	8	3	3	3	1	1	1	1	1	1	1	1	1	1	1	1	
12	8	3	3	3	1	1	1	1	1	1	1	1	1	1	1	1	
13	10	4	4	3	1	1	1	1	1	1	1	1	1	1	1	1	
14	10	4	4	3	1	1	1	1	1	1	1	1	1	1	1	1	
15	11	5	4	3	1	1	1	1	1	1	1	1	1	1	1	1	
16	12	5	3	2	0	0	0	0	0	0	0	0	0	0	0	0	
17	15	7	4	4	1	1	1	1	1	1	1	1	1	1	0	0	
18	16	7	5	4	1	1	1	1	1	1	1	1	1	1	0	0	
19	16	8	4	4	1	1	1	1	1	1	1	1	1	1	0	0	
20	14	8	4	3	1	1	1	1	1	1	1	1	1	1	0	0	
21	13	8	4	3	1	1	1	1	1	1	1	1	1	1	0	0	
22	21	9	5	2	1	1	1	1	1	1	1	1	1	0	0	0	
23	24	10	6	2	1	1	1	1	1	1	1	1	1	0	0	0	
24	25	11	6	3	2	1	1	1	1	1	1	1	1	0	0	0	
25	22	10	8	5	4	3	3	3	3	2	2	2	0	0	0	0	
26	23	12	8	6	4	3	3	3	3	2	2	1	0	0	0	0	
27	25	13	7	5	4	3	2	2	2	2	2	1	0	0	0	0	
28	26	12	8	7	5	3	2	2	2	2	2	1	0	0	0	0	
29	29	14	10	7	5	3	2	2	2	1	1	1	0	0	0	0	
30	31	15	10	8	5	3	2	2	2	1	1	1	0	0	0	0	
31	33	16	11	8	6	4	4	2	2	1	1	1	1	1	0	0	
32	37	18	12	8	6	4	4	3	3	1	1	1	1	1	1	0	
33	43	20	15	8	6	5	4	3	2	1	1	1	1	1	0	0	
34	44	22	16	9	8	6	5	4	3	2	2	1	1	1	0	0	
35	46	24	16	10	8	6	5	4	1	1	1	1	1	1	1	1	
36	45	24	15	10	8	6	5	4	1	1	1	1	1	1	1	1	
37	40	23	15	8	5	4	3	2	0	0	0	0	0	0	0	0	
38	38	22	15	9	6	4	3	2	0	0	0	0	0	0	0	0	
39	45	29	18	12	8	5	4	2	0	0	0	0	0	0	0	0	
40	51	34	22	15	10	4	4	2	0	0	0	0	0	0	0	0	
41	48	34	19	13	9	4	4	2	1	0	0	0	0	0	0	0	
42	57	37	22	14	9	6	4	2	1	0	0	0	0	0	0	0	
43	60	37	22	14	11	7	4	3	2	0	0	0	0	0	0	0	
44	61	38	27	13	10	5	3	2	2	0	0	0	0	0	0	0	
45	67	43	30	16	12	6	3	2	1	0	0	0	0	0	0	0	
46	77	50	29	18	11	8	5	2	1	0	0	0	0	0	0	0	
47	78	54	31	22	13	10	5	2	1	0	0	0	0	0	0	0	
48	82	57	31	20	12	8	3	2	0	0	0	0	0	0	0	0	
49	81	54	34	24	13	10	3	2	0	0	0	0	0	0	0	0	

ENERGY DISTRIBUTIONS

NUMBER OF COLLISIONS	NUMBER OF UNDISSOCIATED MOLECULES WITH ENERGIES GREATER THAN -																
*****	.17 *****	.18 *****	.19 *****	.20 *****	.21 *****	.22 *****	.23 *****	.24 *****	.25 *****	.26 *****	.27 *****	.28 *****	.29 *****	.30 *****	.31 *****	.32 *****	*****
50	86	55	31	19	9	8	4	2	0	0	0	0	0	0	0	0	
51	90	59	38	23	11	8	2	2	0	0	0	0	0	0	0	0	
52	94	62	38	22	13	9	3	2	1	0	0	0	0	0	0	0	
53	93	58	37	21	13	9	4	3	1	0	0	0	0	0	0	0	
54	95	60	40	24	16	10	5	3	2	2	1	1	1	0	0	0	
55	104	62	42	26	16	11	6	4	3	2	1	1	1	0	0	0	
56	114	69	45	27	17	11	6	4	3	2	1	1	1	0	0	0	
57	119	75	45	31	20	14	8	7	4	3	2	2	2	1	1	1	
58	117	77	47	33	21	15	9	6	4	3	2	2	2	0	0	0	
59	122	84	58	40	26	16	9	7	5	4	3	2	2	1	0	0	
60	129	86	61	41	30	19	13	9	8	6	3	2	1	0	0	0	
61	134	100	67	43	29	18	13	10	8	7	4	2	1	0	0	0	
62	148	109	73	50	37	23	16	13	10	8	5	3	2	1	0	0	
63	156	113	73	56	39	24	19	14	8	7	5	3	2	1	1	1	
64	155	112	77	61	43	26	18	13	8	7	5	3	2	1	1	1	
65	158	110	81	66	43	28	19	13	9	8	5	4	2	1	1	1	
66	159	109	75	61	43	31	21	16	10	9	5	3	3	1	1	1	
67	167	119	84	66	48	33	21	16	10	7	4	4	4	1	1	1	
68	173	122	87	64	45	32	20	19	11	7	5	4	4	2	2	2	
69	169	124	91	63	45	33	19	18	10	6	5	4	4	1	1	1	
70	165	120	93	69	52	37	23	19	11	7	6	5	3	2	1	1	
71	170	121	92	64	52	39	25	17	11	7	6	5	3	2	1	0	
72	179	132	97	66	54	42	26	17	12	8	7	6	2	2	1	0	
73	180	135	98	66	52	40	27	16	14	10	7	6	3	3	2	1	
74	191	142	103	76	57	44	27	18	13	11	9	7	4	4	3	1	
75	191	144	108	80	62	49	30	21	17	12	6	5	3	3	2	1	
76	202	150	106	78	61	45	32	20	15	12	6	5	3	3	2	1	
77	201	145	106	77	59	43	34	24	17	10	6	5	3	3	2	1	
78	211	154	109	83	60	46	35	27	19	12	8	7	5	4	2	2	
79	220	158	116	85	63	47	36	25	18	12	7	5	4	3	2	1	
80	221	157	115	85	65	49	38	27	19	12	7	5	4	4	2	1	
81	234	162	117	87	64	46	35	26	18	11	7	5	3	3	2	1	
82	235	162	118	94	68	48	35	27	19	10	6	4	3	3	2	1	
83	233	168	122	93	69	47	34	27	18	11	6	5	3	3	2	1	
84	242	169	125	98	74	49	34	25	18	11	6	4	2	2	1	0	
85	249	176	128	102	78	52	39	28	20	13	8	5	3	3	2	1	
86	253	182	132	103	78	55	44	28	20	16	9	5	3	3	2	0	
87	254	177	136	102	76	52	44	29	24	19	12	8	3	3	2	0	
88	253	181	138	103	75	54	45	31	25	20	13	9	3	3	3	1	
89	254	188	139	99	72	52	43	28	22	17	13	10	3	3	2	1	
90	257	193	141	99	73	56	45	35	25	21	14	12	5	4	3	2	
91	259	194	142	105	76	57	47	37	26	21	15	12	6	5	4	3	
92	259	193	149	108	82	61	44	34	26	18	13	10	7	3	3	1	
93	269	196	145	104	78	60	44	32	26	19	15	11	8	4	3	1	
94	275	198	150	105	80	59	43	31	25	16	14	11	8	5	4	1	
95	290	206	147	108	84	62	47	34	26	19	17	14	9	8	3	1	
96	287	208	151	113	87	65	48	35	27	19	15	12	9	6	3	1	
97	287	204	149	120	93	70	54	38	28	20	17	13	7	5	2	1	
98	286	205	152	113	85	67	54	38	28	20	17	12	7	4	3	2	
99	287	210	151	113	88	70	54	41	31	22	18	13	7	4	4	2	

ENERGY DISTRIBUTIONS

NUMBER OF COLLISIONS	NUMBER OF UNDISSOCIATED MOLECULES WITH ENERGIES GREATER THAN -																
*****	.17 *****	.18 *****	.19 *****	.20 *****	.21 *****	.22 *****	.23 *****	.24 *****	.25 *****	.26 *****	.27 *****	.28 *****	.29 *****	.30 *****	.31 *****	.32 *****	*****
100	289	217	149	116	90	73	55	42	34	24	18	13	6	4	4	2	
101	316	230	156	116	90	75	53	43	32	23	17	14	7	4	4	2	
102	323	232	164	124	92	72	50	42	32	25	16	14	10	6	6	3	
103	325	225	166	125	94	72	53	48	35	27	14	11	9	4	4	2	
104	331	237	179	128	98	76	53	48	35	29	14	11	9	4	3	2	
105	322	233	169	127	99	75	55	50	35	28	15	11	9	5	3	2	
106	321	238	175	135	103	78	58	52	36	29	15	11	8	4	2	2	
107	329	249	182	137	108	79	59	49	38	28	16	12	8	4	3	3	
108	335	257	185	141	109	85	62	50	37	27	15	13	10	6	5	5	
109	326	255	176	131	102	83	67	50	35	25	15	13	9	7	4	4	
110	334	262	178	133	104	83	65	49	33	26	15	13	9	8	5	5	
111	338	268	191	145	117	87	69	56	35	27	17	15	10	8	6	6	
112	340	261	186	146	117	89	72	57	38	27	19	14	10	9	7	6	
113	344	270	190	156	118	86	62	49	32	26	17	12	10	9	6	6	
114	346	268	191	152	117	87	59	46	30	23	16	11	9	8	5	5	
115	357	274	198	150	119	81	57	42	28	21	16	13	10	8	6	6	
116	351	267	203	159	121	84	56	43	29	21	16	13	9	6	4	3	
117	348	273	209	166	123	87	58	46	33	24	19	16	10	6	5	3	
118	355	280	213	160	123	90	59	47	32	23	17	16	11	6	6	4	
119	358	278	212	154	115	86	55	41	32	24	18	16	10	6	5	5	
120	355	278	215	152	110	86	63	45	33	25	17	16	11	7	6	5	
121	365	279	225	164	117	88	64	41	33	23	19	17	12	8	6	5	
122	367	285	227	169	125	90	66	44	34	23	17	15	11	8	5	4	
123	365	288	228	171	132	93	67	44	33	23	17	15	10	7	5	4	
124	374	296	224	173	126	87	67	47	36	25	15	14	11	8	6	4	
125	387	309	233	180	128	93	71	52	37	28	17	14	12	7	6	4	
126	401	315	239	176	122	87	64	47	38	25	18	14	10	8	6	3	
127	395	314	242	179	126	91	64	47	38	25	18	14	10	8	6	3	
128	404	320	244	179	126	90	65	46	38	23	20	16	10	7	5	4	
129	403	314	241	184	137	98	70	49	39	25	20	16	10	7	5	4	
130	404	312	242	185	137	98	68	44	35	23	17	12	8	5	3	2	
131	413	311	235	182	132	95	68	47	36	27	16	11	7	4	3	2	
132	415	311	237	180	128	95	69	52	39	28	19	12	9	6	4	2	
133	427	313	239	184	123	91	70	52	37	29	17	11	7	4	3	3	
134	422	312	229	179	126	98	74	54	39	29	16	10	7	4	3	2	
135	421	320	234	177	125	101	79	58	41	29	15	11	9	5	3	2	
136	416	313	231	170	125	99	74	58	38	29	18	15	12	8	5	3	
137	426	320	244	178	123	90	70	54	38	30	18	14	12	5	3	1	
138	434	313	245	177	124	91	69	53	37	27	16	15	11	5	2	1	
139	430	312	245	180	127	95	68	50	32	25	15	12	8	4	2	0	
140	431	317	247	175	125	98	70	54	35	28	17	14	6	3	2	1	
141	439	326	244	179	130	97	68	49	33	27	17	12	4	2	2	2	
142	435	336	241	178	128	91	63	51	36	28	20	16	7	4	3	3	
143	428	333	236	178	125	90	59	46	32	25	16	12	4	3	2	2	
144	423	340	249	187	139	102	68	51	35	23	14	11	5	4	3	3	
145	429	338	250	186	135	98	68	50	32	21	15	10	5	4	4	4	
146	425	340	245	183	139	101	68	49	31	21	16	10	6	5	4	4	
147	434	343	248	181	143	101	73	53	36	23	17	10	6	5	4	4	
148	435	339	250	181	140	97	77	55	34	24	18	12	8	7	6	6	
149	432	339	255	187	148	98	78	52	34	25	16	14	11	7	6	5	

ENERGY DISTRIBUTIONS

NUMBER OF COLLISIONS	NUMBER OF UNDISSOCIATED MOLECULES WITH ENERGIES GREATER THAN -															
*****	.17 *****	.18 *****	.19 *****	.20 *****	.21 *****	.22 *****	.23 *****	.24 *****	.25 *****	.26 *****	.27 *****	.28 *****	.29 *****	.30 *****	.31 *****	.32 *****	*****
150	434	342	252	186	149	100	77	50	35	26	17	14	10	7	7	6	
151	445	346	250	188	148	102	77	49	34	27	18	14	9	8	7	5	
152	455	351	253	189	151	109	78	52	38	30	20	16	11	10	9	5	
153	455	356	250	193	157	118	81	52	35	25	17	15	11	10	9	6	
154	455	356	262	205	159	119	80	49	34	24	16	16	11	9	8	5	
155	469	358	265	203	157	113	79	50	34	25	17	16	11	8	8	6	
156	456	348	258	203	160	116	80	54	33	21	15	14	10	9	8	5	
157	466	360	267	208	162	115	77	50	33	22	17	16	10	9	8	6	
158	458	349	261	195	153	110	77	50	33	23	16	13	9	8	8	7	
159	463	350	254	185	141	103	70	48	32	22	14	12	8	7	7	6	
160	462	345	249	183	142	105	73	53	31	23	17	14	10	9	7	6	
161	475	357	269	196	149	107	76	54	31	24	17	13	9	8	6	6	
162	480	358	270	195	153	116	76	50	35	25	18	16	13	10	6	6	
163	481	360	274	203	156	113	76	51	33	23	16	11	11	10	8	7	
164	471	358	274	210	162	120	81	56	36	27	18	13	13	11	9	7	
165	461	354	265	207	166	124	80	52	36	28	19	13	12	10	9	8	
166	462	360	266	210	167	124	83	55	36	27	19	14	13	10	9	8	
167	462	360	265	210	161	121	84	60	38	30	21	16	14	10	9	9	
168	483	373	269	206	158	120	88	63	43	33	23	17	15	10	9	9	
169	482	385	290	216	163	117	90	63	44	35	24	17	17	10	9	8	
170	475	377	283	212	159	117	90	63	42	34	22	16	16	11	9	8	
171	482	377	286	210	152	116	89	65	47	35	24	18	18	14	12	9	
172	503	387	284	209	151	109	85	67	47	34	24	19	18	14	12	10	
173	501	387	295	220	158	118	83	68	44	32	22	19	18	14	12	10	
174	498	390	304	227	166	119	88	72	51	39	27	23	19	16	13	10	
175	510	409	318	236	164	120	86	70	49	37	27	23	19	16	13	10	
176	512	410	315	232	167	120	84	73	50	38	27	21	18	14	12	9	
177	510	409	314	236	166	126	91	80	53	40	30	22	19	14	13	11	
178	520	416	323	236	171	129	93	79	56	39	30	25	20	16	14	12	
179	530	415	325	234	167	133	92	79	56	41	30	24	20	15	13	12	
180	533	404	320	232	165	129	89	74	53	38	29	23	17	13	10	10	
181	544	403	320	243	168	130	93	77	56	36	28	19	17	14	11	10	
182	531	396	322	243	174	133	99	79	57	37	30	20	17	13	12	11	
183	530	384	315	236	173	129	95	78	57	40	32	21	14	13	12	11	
184	525	396	316	239	179	132	101	74	55	40	31	22	14	13	12	11	
185	524	403	315	242	173	128	96	74	56	40	35	24	15	14	13	11	
186	529	409	314	250	182	138	98	75	55	39	33	21	16	13	12	10	
187	534	416	319	251	188	141	103	79	60	39	33	21	16	14	11	11	
188	543	430	327	248	202	153	105	79	59	40	33	18	14	12	10	10	
189	556	434	324	253	196	147	105	81	61	38	29	16	13	11	10	9	
190	548	433	324	249	195	147	104	80	59	41	31	17	13	11	10	8	
191	552	440	332	245	193	149	115	81	63	43	34	23	17	14	12	10	
192	571	452	341	257	202	152	117	89	67	46	37	24	16	14	12	8	
193	570	451	344	264	207	161	124	89	65	45	34	22	16	12	10	7	
194	565	445	335	258	196	151	118	83	60	41	32	22	17	14	12	8	
195	578	448	336	252	191	151	118	81	61	41	34	26	19	15	12	8	
196	578	443	336	245	185	145	117	80	62	46	34	27	19	14	12	7	
197	575	447	336	246	186	142	114	75	62	45	33	25	19	14	11	8	
198	587	452	330	247	188	146	115	78	58	47	33	27	22	14	10	7	
199	594	456	337	250	196	151	120	86	65	50	33	25	20	14	10	6	

ENERGY DISTRIBUTIONS

NUMBER OF COLLISIONS	NUMBER OF UNDISSOCIATED MOLECULES WITH ENERGIES GREATER THAN -																
*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
200	596	457	342	263	209	157	126	89	64	49	35	29	22	13	10	6	

ANGULAR MOMENTUM DISTRIBUTIONS

NUMBER OF COLLISIONS	NUMBER OF UNDISSOCIATED MOLECULES WITH ANGULAR MOMENTUM SQUARED GREATER THAN -														
	.0	.1	.2	.3	.4	.5	.6	.7	.8	.9	1.0	1.5	2.0	2.5	3.0
0	10000	7043	5013	3519	2470	1747	1223	877	633	452	329	53	8	2	0
1	10000	7270	5515	4202	3160	2414	1879	1506	1199	946	785	301	106	46	7
2	10000	7465	5918	4689	3720	2960	2391	2010	1688	1392	1194	528	218	100	33
3	10000	7658	6242	5105	4155	3388	2821	2401	2058	1730	1511	714	320	151	62
4	10000	7828	6558	5494	4598	3869	3283	2842	2461	2097	1864	940	453	220	98
5	10000	7994	6820	5793	4963	4254	3674	3221	2805	2449	2198	1137	569	289	146
6	10000	8129	7046	6076	5275	4598	4021	3571	3145	2791	2516	1376	712	361	183
7	10000	8244	7241	6338	5564	4900	4338	3870	3422	3037	2733	1528	813	425	217
8	10000	8340	7381	6545	5835	5197	4620	4153	3702	3287	2983	1727	972	521	282
9	10000	8452	7583	6780	6104	5492	4921	4425	3982	3576	3243	1901	1079	616	345
10	10000	8543	7700	6938	6248	5659	5116	4646	4183	3746	3399	2081	1207	706	402
11	10000	8605	7804	7077	6391	5809	5278	4817	4387	3942	3582	2233	1337	797	454
12	10000	8679	7908	7208	6569	6025	5481	4999	4549	4118	3756	2402	1461	873	501
13	10000	8704	7959	7281	6675	6155	5607	5166	4729	4297	3933	2578	1584	947	564
14	10000	8765	8042	7408	6812	6306	5760	5303	4861	4453	4085	2705	1691	1009	619
15	10000	8839	8103	7483	6894	6392	5873	5415	4979	4586	4221	2804	1773	1093	679
16	9999	8874	8151	7527	6968	6472	5981	5536	5101	4707	4353	2885	1860	1181	752
17	9999	8935	8224	7600	7056	6556	6067	5631	5208	4804	4437	2991	1930	1264	788
18	9999	8927	8264	7651	7107	6604	6128	5702	5280	4881	4513	3060	2004	1314	844
19	9999	8984	8338	7748	7216	6683	6223	5798	5380	4994	4621	3134	2052	1367	906
20	9999	9005	8388	7771	7264	6754	6304	5896	5475	5086	4711	3236	2136	1424	943
21	9999	9056	8444	7873	7375	6856	6393	6010	5581	5175	4824	3348	2234	1467	981
22	9999	9056	8463	7917	7419	6919	6451	6041	5602	5225	4861	3380	2277	1511	1013
23	9999	9041	8446	7926	7418	6928	6465	6069	5620	5259	4916	3456	2361	1561	1077
24	9999	9078	8489	7977	7460	6988	6534	6154	5715	5362	4989	3496	2407	1611	1103
25	9999	9118	8541	8039	7517	7037	6589	6209	5755	5378	5012	3548	2440	1655	1132
26	9999	9109	8551	8044	7544	7062	6649	6250	5813	5430	5077	3636	2508	1713	1182
27	9999	9147	8618	8116	7606	7116	6718	6324	5902	5521	5179	3708	2589	1809	1221
28	9999	9148	8635	8133	7660	7180	6786	6392	5968	5601	5270	3796	2678	1872	1278
29	9999	9180	8665	8177	7691	7221	6817	6422	5995	5605	5265	3796	2682	1903	1291
30	9999	9237	8725	8224	7754	7303	6870	6462	6022	5642	5291	3837	2716	1935	1316
31	9999	9234	8727	8240	7780	7330	6908	6517	6086	5687	5354	3881	2747	1944	1326
32	9999	9236	8730	8244	7808	7340	6905	6517	6109	5722	5383	3924	2792	1983	1370
33	9999	9251	8742	8274	7811	7356	6939	6550	6162	5791	5448	3929	2769	1962	1358
34	9999	9284	8787	8327	7851	7417	7006	6608	6229	5847	5491	3966	2822	2013	1392
35	9999	9295	8798	8329	7903	7471	7045	6647	6263	5870	5509	3999	2839	2038	1416
36	9999	9317	8823	8363	7936	7502	7075	6658	6278	5873	5540	4010	2824	2011	1397
37	9998	9323	8852	8407	7969	7513	7100	6691	6323	5936	5601	4071	2852	2013	1410
38	9998	9304	8846	8409	7968	7532	7139	6735	6360	5954	5642	4117	2887	2039	1471
39	9998	9302	8871	8429	8013	7572	7184	6759	6394	5983	5653	4140	2916	2080	1506
40	9998	9321	8881	8441	8026	7589	7222	6786	6427	5998	5672	4204	2981	2138	1536
41	9998	9318	8874	8450	8050	7643	7260	6842	6467	6052	5717	4218	3030	2163	1563
42	9998	9336	8881	8446	8057	7632	7244	6845	6452	6056	5724	4230	3053	2191	1545
43	9998	9324	8883	8465	8073	7667	7270	6857	6473	6078	5750	4230	3059	2190	1580
44	9998	9346	8916	8514	8097	7687	7295	6902	6542	6130	5811	4260	3108	2235	1614
45	9998	9376	8953	8528	8106	7694	7311	6921	6556	6156	5830	4297	3162	2285	1663
46	9998	9379	8935	8524	8115	7738	7350	6962	6582	6187	5855	4346	3171	2308	1686
47	9998	9387	8947	8517	8123	7751	7390	7001	6641	6241	5902	4357	3199	2318	1679
48	9998	9390	8959	8506	8112	7738	7388	7008	6676	6297	5930	4399	3235	2337	1676
49	9998	9405	8976	8549	8135	7783	7408	7014	6702	6354	5983	4465	3267	2361	1702

ANGULAR MOMENTUM DISTRIBUTIONS

NUMBER OF COLLISIONS	NUMBER OF UNDISSOCIATED MOLECULES WITH ANGULAR MOMENTUM SQUARED GREATER THAN -														
*****	.0	.1	.2	.3	.4	.5	.6	.7	.8	.9	1.0	1.5	2.0	2.5	3.0
	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****	*****
50	9958	9401	8981	8557	8154	7775	7424	7044	6711	6348	5994	4487	3271	2370	1718
51	9958	9371	8977	8553	8169	7788	7446	7064	6721	6338	5986	4508	3288	2382	1714
52	9958	9355	8955	8543	8159	7780	7429	7080	6707	6345	5986	4512	3294	2384	1730
53	9958	9389	8990	8557	8162	7835	7457	7110	6729	6352	6012	4559	3334	2412	1751
54	9958	9387	8979	8561	8168	7841	7462	7125	6777	6379	6039	4584	3386	2475	1798
55	9958	9412	8986	8581	8178	7851	7454	7128	6777	6396	6056	4656	3418	2509	1821
56	9958	9404	8966	8560	8160	7840	7449	7108	6764	6394	6043	4659	3436	2508	1831
57	9958	9418	8984	8561	8146	7821	7440	7098	6751	6395	6044	4685	3454	2540	1859
58	9957	9417	8973	8567	8171	7830	7485	7141	6802	6452	6089	4711	3465	2543	1888
59	9957	9418	8980	8599	8191	7846	7476	7133	6794	6454	6103	4717	3479	2545	1891
60	9957	9434	9002	8611	8208	7835	7459	7116	6773	6443	6079	4671	3455	2544	1863
61	9957	9433	9013	8631	8259	7868	7487	7137	6781	6429	6079	4682	3455	2534	1894
62	9957	9426	9012	8638	8274	7863	7479	7151	6781	6416	6051	4636	3427	2550	1883
63	9957	9398	9005	8618	8243	7872	7505	7163	6798	6421	6061	4624	3451	2571	1888
64	9957	9422	9025	8624	8237	7835	7481	7154	6800	6453	6091	4644	3487	2587	1909
65	9957	9442	9017	8628	8242	7854	7490	7165	6816	6471	6127	4653	3499	2607	1943
66	9957	9453	9017	8617	8258	7855	7493	7173	6816	6474	6144	4645	3512	2622	1935
67	9957	9455	9000	8595	8225	7833	7469	7175	6820	6483	6146	4680	3530	2631	1936
68	9957	9462	9004	8610	8245	7855	7506	7189	6849	6516	6177	4735	3583	2673	1988
69	9956	9475	9026	8627	8243	7872	7533	7176	6832	6507	6185	4746	3568	2689	2014
70	9956	9476	9014	8638	8251	7870	7519	7172	6835	6509	6166	4758	3587	2675	2008
71	9956	9449	9009	8639	8250	7872	7515	7172	6842	6520	6184	4787	3611	2688	2010
72	9956	9450	9034	8656	8243	7879	7538	7199	6872	6534	6206	4821	3647	2709	2014
73	9956	9434	9018	8640	8241	7861	7526	7174	6855	6496	6157	4799	3626	2695	1973
74	9956	9457	9037	8673	8295	7896	7567	7226	6902	6531	6205	4805	3634	2685	1972
75	9956	9455	9040	8652	8287	7904	7575	7249	6923	6539	6200	4812	3643	2706	2028
76	9956	9457	9033	8646	8287	7917	7547	7214	6875	6510	6185	4797	3632	2706	2018
77	9956	9476	9057	8643	8275	7935	7561	7211	6849	6490	6148	4787	3660	2735	2025
78	9956	9447	9054	8628	8253	7895	7544	7204	6882	6532	6185	4809	3680	2753	2002
79	9955	9438	9038	8626	8267	7903	7550	7214	6883	6556	6215	4785	3682	2755	2045
80	9955	9437	9064	8675	8302	7928	7578	7225	6903	6577	6255	4789	3670	2751	2030
81	9955	9436	9047	8655	8289	7911	7560	7219	6913	6572	6264	4810	3684	2752	2039
82	9955	9433	9057	8659	8295	7927	7565	7240	6923	6607	6301	4865	3725	2801	2083
83	9955	9470	9071	8689	8319	7969	7627	7297	6925	6595	6297	4899	3734	2816	2092
84	9954	9493	9078	8680	8324	7989	7656	7327	6978	6645	6334	4898	3712	2815	2107
85	9954	9493	9092	8734	8363	8024	7691	7353	7026	6686	6369	4903	3716	2844	2091
86	9953	9501	9098	8738	8365	8024	7679	7327	6992	6651	6321	4886	3699	2830	2090
87	9953	9509	9086	8718	8343	7992	7646	7273	6955	6610	6267	4843	3691	2822	2087
88	9953	9512	9109	8737	8357	8000	7658	7286	6956	6598	6264	4861	3689	2815	2082
89	9952	9506	9113	8760	8376	8024	7659	7289	6947	6591	6275	4874	3656	2801	2090
90	9952	9511	9127	8762	8404	8040	7683	7321	6971	6614	6292	4917	3708	2830	2122
91	9952	9499	9123	8735	8379	8031	7690	7318	6952	6618	6291	4907	3713	2835	2139
92	9951	9481	9095	8737	8382	8043	7689	7339	6983	6615	6307	4945	3772	2851	2174
93	9951	9508	9128	8767	8409	8053	7695	7337	7014	6625	6315	4922	3766	2839	2175
94	9951	9510	9136	8782	8429	8082	7725	7376	7038	6649	6333	4926	3773	2850	2156
95	9951	9520	9151	8787	8424	8071	7733	7392	7051	6651	6318	4958	3779	2863	2176
96	9951	9522	9158	8796	8432	8069	7733	7395	7048	6649	6335	4952	3824	2901	2176
97	9951	9538	9153	8798	8426	8069	7722	7379	7040	6685	6363	4947	3823	2888	2176
98	9951	9541	9166	8817	8463	8077	7722	7374	7053	6712	6373	5002	3857	2925	2178
99	9951	9531	9171	8839	8474	8104	7739	7369	7044	6720	6384	5012	3864	2930	2190

ANGULAR MOMENTUM DISTRIBUTIONS

NUMBER OF COLLISIONS	NUMBER OF UNDISSOCIATED MOLECULES WITH ANGULAR MOMENTUM SQUARED GREATER THAN -														
*****	.0	.1	.2	.3	.4	.5	.6	.7	.8	.9	1.0	1.5	2.0	2.5	3.0
100	9951	9520	9177	8818	8456	8085	7745	7389	7062	6750	6418	5047	3867	2919	2197
101	9951	9512	9184	8802	8452	8097	7767	7422	7096	6782	6458	5081	3883	2951	2234
102	9951	9516	9174	8783	8450	8116	7771	7411	7064	6769	6446	5046	3866	2931	2205
103	9950	9536	9201	8810	8456	8151	7805	7429	7108	6797	6479	5070	3880	2964	2237
104	9950	9550	9200	8802	8426	8117	7784	7409	7069	6751	6438	5030	3865	2961	2246
105	9950	9545	9209	8835	8469	8148	7844	7459	7113	6768	6437	4989	3814	2937	2231
106	9950	9552	9203	8835	8493	8174	7837	7465	7122	6767	6440	4999	3814	2943	2225
107	9950	9541	9183	8832	8492	8171	7827	7484	7124	6779	6455	5038	3851	2958	2244
108	9950	9524	9157	8811	8461	8120	7777	7452	7100	6740	6425	5008	3842	2943	2244
109	9989	9517	9148	8827	8488	8145	7785	7447	7085	6746	6420	5013	3844	2963	2259
110	9989	9511	9157	8817	8459	8112	7789	7444	7072	6724	6375	5003	3859	2982	2279
111	9989	9523	9161	8817	8458	8132	7828	7482	7133	6766	6422	5026	3901	3022	2297
112	9989	9533	9184	8844	8498	8153	7843	7504	7143	6788	6456	5063	3902	2982	2282
113	9989	9507	9149	8810	8458	8126	7821	7471	7114	6767	6426	5058	3916	2984	2286
114	9988	9521	9159	8830	8475	8142	7837	7461	7111	6782	6452	5091	3960	3001	2295
115	9988	9519	9151	8819	8467	8124	7816	7465	7095	6766	6447	5079	3948	3016	2304
116	9986	9537	9155	8805	8463	8123	7807	7486	7134	6805	6488	5089	3938	3016	2285
117	9986	9552	9183	8827	8478	8138	7811	7488	7123	6784	6467	5065	3931	2998	2319
118	9986	9556	9195	8866	8526	8173	7850	7520	7152	6820	6494	5089	3921	2998	2321
119	9985	9574	9203	8866	8539	8204	7862	7521	7188	6839	6492	5074	3939	3025	2340
120	9985	9584	9191	8860	8516	8192	7829	7474	7146	6801	6447	5061	3940	3039	2288
121	9985	9577	9209	8896	8573	8240	7899	7544	7199	6838	6480	5079	3954	3034	2312
122	9984	9577	9201	8880	8546	8218	7882	7539	7207	6853	6481	5093	3995	3056	2348
123	9984	9549	9195	8866	8514	8199	7859	7519	7186	6835	6476	5038	3937	3014	2332
124	9984	9547	9168	8866	8511	8204	7858	7506	7186	6821	6457	5050	3939	3029	2329
125	9984	9545	9202	8868	8538	8211	7867	7524	7211	6840	6497	5075	3934	3014	2296
126	9983	9546	9189	8843	8506	8189	7855	7521	7194	6845	6502	5094	3949	3027	2313
127	9983	9551	9203	8863	8532	8218	7856	7510	7187	6852	6509	5090	3926	3011	2294
128	9982	9537	9190	8848	8547	8203	7853	7518	7193	6856	6520	5092	3919	3004	2288
129	9981	9542	9188	8847	8524	8182	7841	7511	7186	6840	6507	5104	3948	3018	2313
130	9979	9546	9198	8862	8542	8202	7869	7520	7182	6842	6500	5118	3955	3046	2326
131	9979	9544	9192	8855	8504	8186	7860	7515	7183	6835	6501	5130	3967	3067	2360
132	9979	9536	9184	8832	8486	8168	7838	7529	7174	6853	6531	5157	4006	3062	2367
133	9979	9540	9167	8803	8458	8144	7807	7505	7150	6815	6477	5086	3965	3062	2346
134	9979	9524	9166	8814	8469	8160	7827	7514	7175	6841	6515	5085	3957	3078	2342
135	9979	9509	9143	8795	8466	8145	7799	7480	7163	6824	6508	5077	3966	3043	2326
136	9979	9539	9162	8802	8475	8162	7831	7505	7159	6837	6522	5069	3964	3045	2347
137	9977	9557	9167	8807	8477	8163	7854	7523	7170	6831	6531	5070	3932	3038	2352
138	9977	9547	9163	8807	8500	8192	7865	7559	7216	6860	6555	5109	3959	3062	2378
139	9976	9538	9138	8784	8449	8154	7829	7533	7208	6861	6543	5104	3942	3043	2370
140	9976	9526	9161	8816	8473	8179	7838	7528	7211	6853	6545	5103	3931	3041	2380
141	9976	9540	9161	8811	8464	8164	7822	7531	7227	6884	6547	5110	3945	3080	2395
142	9976	9530	9143	8798	8462	8136	7788	7484	7179	6850	6528	5078	3931	3044	2369
143	9975	9542	9146	8789	8464	8121	7780	7464	7151	6820	6508	5065	3950	3043	2381
144	9975	9553	9165	8813	8497	8146	7800	7491	7183	6862	6518	5075	3962	3045	2349
145	9974	9545	9164	8815	8487	8137	7775	7447	7134	6823	6485	5105	3984	3060	2355
146	9974	9550	9168	8803	8461	8124	7768	7453	7106	6798	6465	5088	3959	3052	2366
147	9974	9523	9149	8774	8443	8117	7783	7481	7145	6821	6479	5091	3988	3056	2375
148	9974	9517	9145	8780	8446	8124	7797	7481	7161	6811	6469	5079	3968	3047	2351
149	9973	9514	9126	8758	8424	8087	7750	7449	7130	6815	6485	5119	3998	3122	2405

ANGULAR MOMENTUM DISTRIBUTIONS

NUMBER OF COLLISIONS	NUMBER OF UNDISSOCIATED MOLECULES WITH ANGULAR MOMENTUM SQUARED GREATER THAN -														
	.0	.1	.2	.3	.4	.5	.6	.7	.8	.9	1.0	1.5	2.0	2.5	3.0
150	9973	9518	9114	8745	8428	8083	7747	7432	7105	6793	6463	5118	3975	3087	2388
151	9972	9526	9119	8761	8412	8052	7730	7429	7116	6792	6462	5117	3975	3091	2408
152	9972	9535	9125	8776	8430	8078	7738	7421	7125	6799	6472	5137	3989	3086	2405
153	9972	9525	9134	8786	8453	8100	7759	7437	7134	6791	6447	5068	3973	3109	2414
154	9971	9515	9136	8790	8458	8119	7764	7424	7106	6780	6444	5062	3979	3115	2401
155	9970	9514	9137	8801	8444	8108	7766	7411	7106	6784	6439	5085	4010	3124	2396
156	9968	9523	9155	8811	8457	8106	7772	7409	7096	6765	6445	5082	3994	3090	2345
157	9968	9516	9169	8827	8470	8108	7758	7387	7077	6738	6418	5079	3977	3083	2332
158	9968	9515	9173	8795	8441	8090	7753	7389	7070	6740	6415	5091	3961	3067	2335
159	9967	9529	9170	8819	8465	8108	7785	7413	7053	6736	6407	5099	3993	3073	2378
160	9967	9535	9185	8837	8494	8131	7783	7414	7056	6741	6421	5068	3921	3046	2357
161	9967	9538	9178	8825	8466	8105	7784	7417	7043	6732	6409	5044	3938	3060	2363
162	9967	9545	9182	8843	8466	8105	7770	7396	7026	6692	6392	5050	3938	3052	2366
163	9967	9527	9164	8837	8480	8108	7761	7414	7051	6709	6389	5058	3958	3072	2391
164	9967	9537	9167	8851	8503	8135	7806	7465	7120	6751	6441	5069	3959	3060	2352
165	9967	9539	9162	8834	8492	8136	7811	7459	7101	6748	6441	5069	3931	3068	2373
166	9967	9537	9133	8825	8480	8141	7797	7458	7113	6762	6452	5063	3924	3036	2335
167	9966	9520	9147	8808	8485	8149	7795	7457	7114	6783	6479	5049	3888	3006	2302
168	9966	9523	9152	8805	8460	8134	7773	7436	7086	6741	6448	5064	3924	3025	2317
169	9965	9519	9123	8771	8447	8120	7776	7449	7090	6762	6434	5077	3936	3047	2330
170	9965	9528	9130	8792	8455	8121	7776	7429	7080	6757	6411	5093	3950	3032	2315
171	9965	9538	9159	8796	8429	8111	7771	7429	7102	6773	6442	5135	3960	3059	2313
172	9965	9523	9143	8776	8421	8106	7766	7439	7122	6789	6477	5155	3978	3084	2329
173	9965	9517	9142	8795	8451	8129	7812	7490	7142	6815	6520	5211	4009	3116	2347
174	9965	9527	9174	8812	8468	8147	7809	7490	7171	6846	6556	5225	3999	3087	2345
175	9965	9539	9185	8822	8471	8146	7810	7476	7171	6836	6539	5210	4017	3099	2380
176	9963	9536	9178	8814	8484	8157	7830	7506	7191	6868	6570	5233	4068	3120	2404
177	9963	9526	9172	8815	8491	8175	7851	7512	7198	6895	6595	5225	4058	3106	2392
178	9963	9528	9198	8844	8550	8217	7905	7548	7242	6933	6627	5246	4065	3092	2383
179	9963	9546	9199	8850	8540	8209	7906	7539	7224	6909	6597	5206	4034	3101	2364
180	9961	9541	9180	8829	8519	8195	7890	7523	7227	6925	6608	5223	4034	3109	2379
181	9960	9545	9186	8837	8525	8198	7897	7544	7241	6921	6612	5244	4073	3146	2413
182	9960	9549	9215	8877	8540	8196	7886	7557	7253	6927	6589	5226	4065	3146	2410
183	9960	9531	9199	8859	8527	8184	7898	7571	7255	6921	6588	5238	4098	3130	2404
184	9960	9536	9197	8865	8534	8173	7865	7542	7241	6914	6587	5243	4094	3128	2416
185	9959	9540	9201	8844	8520	8170	7860	7554	7237	6909	6582	5225	4064	3117	2411
186	9957	9532	9191	8851	8540	8182	7857	7534	7220	6870	6552	5212	4056	3115	2427
187	9957	9528	9186	8851	8550	8192	7871	7541	7217	6844	6517	5185	4024	3068	2384
188	9956	9526	9186	8851	8525	8179	7857	7551	7247	6874	6553	5184	4033	3074	2351
189	9955	9527	9191	8851	8512	8183	7870	7585	7290	6898	6575	5180	4062	3079	2378
190	9954	9524	9185	8842	8514	8194	7873	7575	7282	6910	6568	5160	4039	3083	2402
191	9954	9548	9199	8862	8505	8167	7854	7569	7265	6918	6553	5158	4007	3094	2397
192	9953	9534	9183	8830	8490	8149	7825	7538	7216	6885	6527	5162	4032	3120	2429
193	9952	9498	9135	8813	8451	8117	7791	7498	7176	6881	6525	5158	4036	3125	2437
194	9952	9509	9137	8810	8466	8109	7781	7474	7144	6836	6489	5095	3959	3096	2418
195	9952	9522	9173	8858	8519	8171	7838	7517	7178	6866	6526	5136	3986	3113	2438
196	9952	9528	9179	8842	8505	8168	7850	7550	7197	6881	6546	5115	3990	3075	2419
197	9951	9534	9184	8854	8514	8174	7855	7541	7186	6860	6536	5124	3980	3067	2423
198	9950	9513	9161	8830	8495	8143	7808	7459	7122	6814	6491	5081	3972	3063	2392
199	9950	9516	9181	8854	8511	8169	7840	7478	7158	6841	6505	5089	3990	3083	2412

ANGULAR MOMENTUM DISTRIBUTIONS

NUMBER OF COLLISIONS	NUMBER OF UNDISSOCIATED MOLECULES WITH ANGULAR MOMENTUM SQUARED GREATER THAN -														
*****	.0 *****	.1 *****	.2 *****	.3 *****	.4 *****	.5 *****	.6 *****	.7 *****	.8 *****	.9 *****	1.0 *****	1.5 *****	2.0 *****	2.5 *****	3.0 *****
200	9950	9528	9201	8856	8524	8191	7869	7504	7174	6855	6524	5087	3973	3087	2407

ANGULAR MOMENTUM DISTRIBUTIONS

NUMBER OF COLLISIONS	NUMBER OF UNDISSOCIATED MOLECULES WITH ANGULAR MOMENTUM SQUARED GREATER THAN -														
*****	3.5 *****	4.0 *****	4.5 *****	5.0 *****	5.5 *****	6.0 *****	6.5 *****	7.0 *****	7.5 *****	8.0 *****	8.5 *****	9.0 *****	9.5 *****	10.0 *****	*****
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
1	5	2	0	0	0	0	0	0	0	0	0	0	0	0	
2	14	4	2	0	0	0	0	0	0	0	0	0	0	0	
3	27	11	7	4	2	1	0	0	0	0	0	0	0	0	
4	48	23	13	6	3	2	1	0	0	0	0	0	0	0	
5	67	31	15	7	4	2	1	0	0	0	0	0	0	0	
6	88	39	26	11	7	4	1	1	0	0	0	0	0	0	
7	101	47	27	15	12	6	3	3	0	0	0	0	0	0	
8	143	72	46	29	18	9	4	4	1	1	1	0	0	0	
9	177	98	62	39	25	9	6	6	2	2	2	1	0	0	
10	217	125	80	53	36	14	5	5	3	3	3	2	1	1	
11	266	157	94	64	36	16	5	4	3	3	3	2	1	1	
12	304	185	114	72	34	18	8	7	4	4	3	2	1	1	
13	330	205	132	85	43	29	16	9	6	5	3	2	1	1	
14	368	230	153	103	53	38	23	14	11	7	2	1	1	1	
15	410	241	163	109	61	36	25	16	12	7	2	1	1	1	
16	444	268	183	117	71	43	26	15	11	7	0	0	0	0	
17	473	294	196	121	77	44	27	15	11	7	4	2	2	2	
18	523	317	210	138	91	52	31	19	12	4	2	1	1	1	
19	576	356	242	159	106	55	36	24	16	5	4	3	1	1	
20	608	382	253	162	110	57	36	25	18	10	5	4	3	3	
21	622	413	269	173	118	65	38	31	19	11	5	4	3	2	
22	638	437	286	184	116	72	42	31	21	13	5	2	1	1	
23	691	474	312	201	134	83	47	34	22	16	7	2	1	1	
24	713	489	326	214	145	92	52	37	24	18	9	2	2	1	
25	757	507	340	219	140	89	51	36	24	17	9	4	3	1	
26	801	537	352	226	143	94	53	37	27	22	11	5	3	2	
27	817	542	368	245	157	102	65	45	32	23	14	9	5	4	
28	835	545	375	258	160	101	65	42	30	19	14	10	6	5	
29	846	551	370	252	162	101	74	47	34	26	18	14	9	7	
30	887	597	409	278	175	118	80	52	37	27	20	14	8	7	
31	914	624	425	290	190	122	81	48	33	24	16	12	6	6	
32	940	647	440	304	202	128	90	55	41	26	18	15	8	6	
33	949	646	451	304	198	130	97	64	51	29	20	15	10	7	
34	967	663	455	304	203	133	100	68	48	25	21	13	9	7	
35	993	688	478	321	226	137	109	73	56	31	24	16	10	7	
36	974	661	478	330	226	137	108	72	54	34	23	12	8	5	
37	996	679	475	321	219	136	106	69	48	28	21	10	7	4	
38	1025	703	490	330	220	140	105	72	48	34	25	17	9	4	
39	1054	739	511	352	227	147	117	75	50	37	27	18	10	5	
40	1074	739	518	370	238	160	122	80	54	38	25	18	10	6	
41	1096	772	540	382	252	174	121	78	53	43	25	17	12	4	
42	1116	774	538	391	260	181	129	84	60	47	28	19	15	6	
43	1132	779	557	403	273	188	139	97	70	52	32	21	16	5	
44	1144	805	572	395	274	186	128	93	69	47	26	15	12	5	
45	1174	822	594	418	296	213	143	105	77	55	30	18	14	6	
46	1195	863	608	433	296	216	145	111	81	58	33	19	15	6	
47	1200	839	591	426	297	211	141	110	75	56	31	18	15	7	
48	1198	840	599	427	292	212	139	101	72	53	32	22	16	9	
49	1220	857	609	432	292	208	146	113	80	58	38	25	17	10	

ANGULAR MOMENTUM DISTRIBUTIONS

NUMBER OF COLLISIONS	NUMBER OF UNDISSOCIATED MOLECULES WITH ANGULAR MOMENTUM SQUARED GREATER THAN -														
*****	3.5 *****	4.0 *****	4.5 *****	5.0 *****	5.5 *****	6.0 *****	6.5 *****	7.0 *****	7.5 *****	8.0 *****	8.5 *****	9.0 *****	9.5 *****	10.0 *****	*****
50	1225	876	622	446	301	219	155	120	81	59	41	26	18	11	
51	1245	880	634	460	317	227	167	127	91	65	49	29	19	11	
52	1233	882	631	463	328	229	165	128	95	70	49	30	20	14	
53	1238	896	633	470	330	229	164	122	93	70	50	33	22	17	
54	1255	916	649	476	346	238	168	133	100	69	48	31	19	16	
55	1278	920	659	474	341	240	175	140	105	76	52	32	21	17	
56	1254	932	656	487	353	255	192	150	112	74	51	31	19	16	
57	1324	969	692	508	366	265	201	153	113	77	54	34	23	19	
58	1350	1000	730	527	378	269	196	142	102	72	51	33	23	20	
59	1374	985	718	522	380	286	213	154	111	81	59	45	33	29	
60	1362	979	708	512	376	294	223	164	118	89	67	52	39	33	
61	1364	978	719	525	374	297	226	161	119	92	69	54	42	34	
62	1370	987	723	528	387	303	235	168	121	94	72	57	44	36	
63	1381	999	722	531	391	297	236	173	128	96	72	49	39	31	
64	1409	1025	740	547	402	297	234	170	124	92	69	47	35	28	
65	1435	1050	785	560	408	308	234	169	120	89	70	52	37	25	
66	1419	1054	782	568	414	309	229	168	118	90	69	54	36	25	
67	1423	1057	782	586	414	308	230	165	116	97	75	54	36	25	
68	1431	1068	799	599	435	323	245	174	123	101	77	53	33	22	
69	1462	1077	797	610	444	328	251	182	128	102	72	49	30	15	
70	1475	1075	805	600	427	312	245	176	123	94	69	48	31	17	
71	1479	1082	801	597	423	307	240	179	124	94	66	46	28	14	
72	1482	1102	798	608	451	335	263	198	142	98	69	50	31	18	
73	1464	1086	807	610	439	325	245	185	135	94	67	50	35	21	
74	1462	1081	799	601	436	315	238	181	131	91	65	53	38	24	
75	1497	1100	807	610	451	316	230	176	126	93	65	52	36	22	
76	1510	1095	797	589	453	317	231	177	127	91	62	49	36	22	
77	1516	1114	804	578	431	309	226	177	129	92	65	54	38	25	
78	1491	1100	808	587	427	305	222	177	134	98	71	51	36	25	
79	1524	1121	821	595	442	326	231	180	131	96	71	49	32	22	
80	1530	1123	841	626	463	348	237	186	133	96	72	53	31	21	
81	1544	1131	844	638	474	353	253	191	137	99	75	53	35	22	
82	1572	1175	872	655	483	368	272	200	150	102	77	50	35	25	
83	1552	1192	889	661	494	374	273	196	145	99	74	53	39	28	
84	1589	1204	886	660	486	372	272	191	142	106	77	60	42	31	
85	1604	1206	888	665	486	362	267	192	144	106	79	61	43	33	
86	1614	1193	884	667	505	375	281	212	155	112	82	61	41	33	
87	1586	1162	875	656	498	370	282	217	164	113	85	61	41	35	
88	1567	1160	865	660	511	386	285	216	157	110	80	61	42	34	
89	1587	1178	879	662	514	382	280	211	163	118	83	63	47	35	
90	1606	1214	901	665	503	386	276	202	157	114	85	65	52	40	
91	1585	1202	881	652	503	382	277	205	160	115	76	56	44	35	
92	1616	1219	896	675	525	396	281	210	159	114	78	55	43	33	
93	1623	1201	894	666	523	395	277	209	156	119	83	62	47	38	
94	1644	1226	904	685	536	395	279	202	159	117	81	61	43	36	
95	1641	1215	907	692	529	403	287	210	158	116	84	62	45	39	
96	1659	1235	908	713	538	406	292	211	158	118	89	67	47	37	
97	1648	1236	916	707	533	410	296	222	168	130	96	68	51	36	
98	1651	1225	895	708	535	414	300	232	178	128	94	68	51	42	
99	1661	1227	907	712	544	418	300	230	174	128	93	70	52	38	

ANGULAR MOMENTUM DISTRIBUTIONS

NUMBER OF COLLISIONS	NUMBER OF UNDISSOCIATED MOLECULES WITH ANGULAR MOMENTUM SQUARED GREATER THAN -														
*****	3.5 *****	4.0 *****	4.5 *****	5.0 *****	5.5 *****	6.0 *****	6.5 *****	7.0 *****	7.5 *****	8.0 *****	8.5 *****	9.0 *****	9.5 *****	10.0 *****	*****
100	1670	1244	930	719	542	412	301	228	179	138	98	70	52	37	
101	1693	1277	958	741	559	428	317	240	186	140	105	78	55	41	
102	1681	1261	949	734	552	426	321	233	181	141	105	78	55	42	
103	1689	1264	960	730	567	438	334	242	187	147	105	77	52	40	
104	1695	1276	960	727	568	436	334	245	189	147	101	80	54	42	
105	1669	1262	961	714	561	427	331	244	187	141	93	71	52	39	
106	1664	1273	968	732	575	437	335	248	194	144	106	80	59	41	
107	1667	1276	957	721	558	425	326	241	191	144	111	82	61	40	
108	1665	1282	973	722	557	435	328	241	185	140	100	80	58	39	
109	1702	1305	971	717	541	417	321	242	193	142	99	78	62	41	
110	1745	1329	986	744	571	435	343	258	199	141	97	76	62	42	
111	1731	1316	975	726	563	426	334	265	206	144	100	83	66	47	
112	1737	1296	971	738	572	434	337	270	205	144	100	85	69	51	
113	1733	1313	980	770	584	438	345	270	198	138	99	85	67	52	
114	1737	1316	996	776	578	439	343	266	195	145	103	90	68	49	
115	1745	1318	1011	763	573	423	338	262	196	144	104	90	65	47	
116	1732	1323	1004	764	571	414	334	247	186	135	102	86	61	48	
117	1753	1345	1005	766	569	420	333	238	176	128	101	85	58	45	
118	1745	1336	1008	777	570	430	331	242	181	140	106	85	62	48	
119	1774	1342	1008	758	570	433	333	242	179	138	105	82	59	46	
120	1752	1327	989	747	564	438	338	243	185	138	102	82	53	42	
121	1758	1322	1015	750	568	433	338	250	190	141	106	83	55	41	
122	1764	1321	994	742	557	428	325	239	179	132	101	79	56	43	
123	1750	1325	997	749	565	422	320	245	180	133	98	72	52	38	
124	1747	1351	1019	764	576	436	329	250	182	140	102	74	51	36	
125	1731	1314	1015	762	597	451	334	254	188	138	98	70	49	37	
126	1753	1331	1015	760	583	431	325	238	175	126	94	67	49	36	
127	1766	1340	1000	738	573	429	328	247	181	131	97	69	52	39	
128	1731	1323	995	734	570	435	328	242	184	125	96	68	55	45	
129	1755	1330	986	741	565	430	330	243	186	126	94	71	57	46	
130	1786	1347	994	752	572	437	340	259	195	139	109	82	62	49	
131	1810	1353	992	748	572	436	332	250	193	140	106	77	58	47	
132	1808	1362	993	756	572	436	328	248	193	144	112	80	62	51	
133	1785	1359	995	753	579	438	321	232	182	136	110	80	58	46	
134	1770	1370	1020	772	591	442	324	227	179	133	104	74	57	47	
135	1774	1380	1021	784	605	450	322	235	179	134	109	80	60	50	
136	1787	1366	1011	759	604	457	333	241	180	136	104	76	54	45	
137	1797	1376	1015	747	594	454	341	256	196	146	117	87	63	47	
138	1803	1375	1021	769	592	452	340	263	194	148	115	82	61	49	
139	1819	1374	1032	782	607	460	349	265	203	139	106	74	56	43	
140	1827	1379	1046	807	618	472	351	256	204	145	108	79	56	44	
141	1813	1364	1037	814	611	456	336	254	210	149	108	80	58	43	
142	1810	1350	1033	807	607	460	348	268	217	154	114	82	63	48	
143	1806	1326	1011	789	595	441	334	260	202	142	99	73	61	48	
144	1810	1338	1022	798	616	460	348	267	206	146	100	71	57	47	
145	1810	1345	1023	807	622	462	345	267	213	149	106	73	55	45	
146	1809	1367	1030	815	623	481	351	273	219	159	114	81	61	49	
147	1812	1387	1036	813	623	482	352	272	219	165	112	82	62	51	
148	1805	1393	1039	815	615	469	348	272	221	167	117	86	60	49	
149	1836	1397	1040	809	615	462	344	276	223	165	115	90	61	50	

ANGULAR MOMENTUM DISTRIBUTIONS

NUMBER OF COLLISIONS	NUMBER OF UNDISSOCIATED MOLECULES WITH ANGULAR MOMENTUM SQUARED GREATER THAN														
*****	3.5	4.0	4.5	5.0	5.5	6.0	6.5	7.0	7.5	8.0	8.5	9.0	9.5	10.0	*****
150	1826	1397	1025	795	608	455	337	265	207	163	116	90	66	51	
151	1847	1413	1039	783	595	434	330	263	206	158	119	93	69	54	
152	1862	1416	1040	780	601	454	344	277	214	163	128	98	71	57	
153	1872	1422	1054	803	603	467	334	274	201	157	126	100	76	62	
154	1851	1407	1048	803	608	465	349	280	207	163	124	100	77	60	
155	1814	1393	1040	787	591	456	348	277	207	160	126	97	73	58	
156	1777	1372	1017	780	582	451	339	265	201	156	117	91	74	59	
157	1783	1346	1008	776	576	450	329	251	187	142	107	86	69	53	
158	1759	1364	1021	790	594	455	339	253	188	137	104	79	64	50	
159	1796	1375	1050	810	616	465	338	246	183	145	109	84	65	48	
160	1818	1408	1061	821	614	453	331	246	190	153	119	88	67	46	
161	1822	1414	1077	841	640	461	344	262	189	153	122	88	67	46	
162	1797	1394	1075	848	648	476	354	276	204	162	121	89	69	45	
163	1829	1416	1071	846	650	470	353	270	213	161	121	93	70	51	
164	1795	1403	1075	864	656	462	349	263	210	157	119	92	69	52	
165	1795	1400	1064	843	645	461	346	259	198	154	121	95	75	59	
166	1776	1382	1050	838	641	467	353	267	205	156	125	101	79	62	
167	1751	1361	1040	823	629	463	344	267	205	153	127	104	75	63	
168	1772	1363	1048	816	618	469	353	264	202	148	131	103	76	59	
169	1803	1403	1066	838	623	470	344	254	197	146	124	97	69	53	
170	1783	1380	1046	815	622	468	345	263	202	153	124	99	71	49	
171	1788	1383	1054	816	611	468	353	266	205	158	125	94	69	49	
172	1755	1396	1060	826	618	480	348	264	205	157	124	89	65	46	
173	1785	1390	1068	825	614	477	360	264	200	146	115	89	65	47	
174	1781	1384	1056	807	605	465	353	260	204	147	109	83	64	45	
175	1802	1404	1068	821	614	471	357	256	196	143	107	78	62	49	
176	1814	1413	1060	809	605	463	349	260	188	137	94	69	53	44	
177	1827	1446	1099	830	613	451	343	259	183	141	92	74	55	43	
178	1840	1445	1104	834	622	470	356	264	186	144	97	75	60	48	
179	1822	1411	1089	839	624	483	367	272	195	151	103	82	65	51	
180	1834	1428	1088	837	632	484	372	275	199	152	104	79	63	50	
181	1878	1463	1101	858	645	507	386	288	205	162	110	86	62	48	
182	1886	1453	1089	839	636	496	365	274	199	147	100	82	60	47	
183	1864	1451	1085	846	644	498	366	272	196	142	93	73	55	47	
184	1863	1426	1068	833	645	495	375	285	205	147	91	73	57	43	
185	1869	1432	1069	833	650	505	376	286	207	147	89	68	57	44	
186	1881	1452	1099	852	644	496	366	280	207	143	94	67	52	40	
187	1837	1438	1100	861	666	502	375	282	202	140	98	72	57	44	
188	1808	1420	1086	857	672	500	377	281	204	146	101	74	56	40	
189	1825	1429	1076	826	645	479	360	268	200	142	95	74	53	41	
190	1831	1422	1074	814	638	475	349	267	202	145	102	78	58	44	
191	1820	1406	1046	784	613	464	350	266	209	148	112	90	66	50	
192	1839	1423	1060	811	613	476	362	279	220	154	123	98	71	56	
193	1862	1416	1084	806	617	482	362	281	219	153	118	93	68	54	
194	1866	1419	1087	806	615	465	346	266	203	139	108	81	58	46	
195	1882	1443	1103	826	622	470	350	268	196	139	111	87	68	51	
196	1867	1429	1094	824	611	470	355	269	194	141	110	87	64	44	
197	1867	1432	1074	805	624	476	360	268	197	142	111	86	61	43	
198	1862	1415	1052	799	620	472	363	273	198	148	112	91	69	45	
199	1852	1421	1068	806	615	467	356	263	192	145	107	89	63	42	

ANGULAR MOMENTUM DISTRIBUTIONS

NUMBER OF COLLISIONS	NUMBER OF UNDISSOCIATED MOLECULES WITH ANGULAR MOMENTUM SQUARED GREATER THAN -														
*****	3.5 *****	4.0 *****	4.5 *****	5.0 *****	5.5 *****	6.0 *****	6.5 *****	7.0 *****	7.5 *****	8.0 *****	8.5 *****	9.0 *****	9.5 *****	10.0 *****	*****
200	1857	1403	1072	819	630	471	367	270	195	153	116	93	64	45	

Special Case of No Angular Momentum Used

NUMBER OF COLLISIONS	NUMBER OF MOLECULES LEFT UNDISSOCIATED	TOTAL ENERGY OF SYSTEM	TOTAL ANGULAR MOMENTUM SQUARED	AVERAGE ENERGY OF UNDISSOCIATED MOLECULES	AVERAGE ANGULAR MOMENTUM SQUARED
0	10000	62.4974813	0	0.624974813E-02	0
10	10000	257.247234	0	0.25724723E-01	0
20	10000	446.984932	0	0.44698493E-01	0
30	10000	630.830246	0	0.63083024E-01	0
40	9999	809.157857	0	0.80889530E-01	0
50	9994	983.350815	0	0.98195057E-01	0
60	9984	1155.08380	0	0.11516380	0
70	9955	1318.40227	0	0.13093501	0
80	9903	1474.92122	0	0.14568309	0
90	9813	1622.59456	0	0.15904503	0
100	9679	1769.15275	0	0.17181417	0
110	9487	1912.16753	0	0.18373284	0
120	9233	2047.70563	0	0.19438594	0
130	8894	2175.90936	0	0.20339174	0
140	8497	2288.52930	0	0.21095851	0
150	8024	2399.91513	0	0.21781398	0
160	7537	2492.74695	0	0.22289676	0
170	7085	2585.77615	0	0.22780865	0
180	6453	2667.92392	0	0.23222586	0
190	5883	2743.39096	0	0.23556514	0
200	5306	2814.12546	0	0.23870155	0
210	4777	2878.22772	0	0.24215374	0
220	4300	2929.75821	0	0.24454144	0
230	3799	2979.97351	0	0.24669622	0
240	3324	3024.73282	0	0.24829840	0
250	2929	3061.62582	0	0.25081772	0
260	2532	3095.68890	0	0.25100635	0
270	2188	3123.34543	0	0.25105993	0
280	1850	3147.96909	0	0.25052546	0
290	1612	3168.88464	0	0.25163181	0
300	1418	3185.99554	0	0.25265117	0
310	1209	3202.91354	0	0.25398114	0
320	1048	3215.87106	0	0.25484359	0
330	924	3226.56363	0	0.25647979	0
340	787	3236.69211	0	0.25660239	0
350	662	3244.17529	0	0.25398822	0
360	569	3251.30658	0	0.25406133	0
370	480	3257.31546	0	0.25297527	0
380	417	3262.02652	0	0.25261701	0
390	360	3266.83395	0	0.25405112	0
400	311	3270.98639	0	0.25581478	0
410	266	3274.10052	0	0.25491285	0
420	228	3277.35455	0	0.25698354	0
430	198	3279.35434	0	0.25709660	0
440	166	3281.78795	0	0.25684622	0
450	135	3283.98727	0	0.25616656	0
460	124	3284.76733	0	0.25759885	0
470	109	3286.15421	0	0.25971684	0
480	89	3287.26981	0	0.25738887	0
490	75	3288.49353	0	0.26076585	0

NUMBER OF COLLISIONS	NUMBER OF MOLECULES LEFT UNDISSOCIATED	TOTAL ENERGY OF SYSTEM	TOTAL ANGULAR MOMENTUM SQUARED	AVERAGE ENERGY OF UNDISSOCIATED MOLECULES	AVERAGE ANGULAR MOMENTUM SQUARED
500	62	3289.48920	0	0.26383688	0
510	58	3289.74274	0	0.26292358	0
520	47	3290.35521	0	0.26109436	0
530	41	3290.72690	0	0.26074088	0
540	36	3290.91470	0	0.25647985	0
550	29	3291.22925	0	0.25139559	0
560	26	3291.25275	0	0.24435087	0
570	23	3291.47772	0	0.24390621	0
580	22	3291.43631	0	0.23801867	0
590	21	3291.78336	0	0.25065763	0
600	18	3292.06335	0	0.25451277	0
610	14	3292.17703	0	0.24272966	0
620	13	3292.24521	0	0.24055557	0
630	12	3292.35440	0	0.24064226	0
640	11	3292.30502	0	0.22895222	0
650	10	3292.48044	0	0.23748419	0
660	10	3292.62589	0	0.25203036	0
670	9	3292.80914	0	0.26088168	0
680	9	3292.89777	0	0.27072228	0
690	6	3293.09579	0	0.27322362	0
700	6	3293.11386	0	0.27622848	0
710	5	3293.16925	0	0.27625171	0
720	3	3293.23422	0	0.26792093	0
730	2	3293.28607	0	0.26751521	0
740	1	3293.29034	0	0.21897896	0
750	1	3293.31668	0	0.24532087	0
760	1	3293.32867	0	0.25729451	0
770	1	3293.33426	0	0.26208467	0
780	1	3293.35406	0	0.28269359	0
790	1	3293.37793	0	0.30655972	0
800	0	3293.39575	0	0	0

ENERGY DISTRIBUTIONS

NUMBER OF COLLISIONS	NUMBER OF UNDISSOCIATED MOLECULES WITH ENERGIES GREATER THAN -																
	.00	.01	.02	.03	.04	.05	.06	.07	.08	.09	.10	.11	.12	.13	.14	.15	. . .
0	10000	1852	248	26	1	0	0	0	0	0	0	0	0	0	0	0	
10	10000	7725	5135	3194	1967	1140	687	400	246	124	69	46	22	17	13	9	
20	10000	9446	8075	6463	4906	3482	2429	1664	1115	711	452	300	192	133	97	62	
30	10000	9879	9350	8438	7248	5897	4609	3473	2589	1902	1347	965	676	464	348	246	1
40	9999	9970	9823	9387	8683	7738	6665	5422	4402	3447	2664	2017	1492	1085	807	598	4
50	9994	9989	9940	9780	9424	8874	8108	7120	6108	5121	4237	3377	2612	2015	1568	1218	9
60	9984	9982	9970	9900	9751	9450	8952	8306	7507	6646	5734	4895	4042	3251	2634	2057	16
70	9955	9955	9951	9936	9865	9724	9452	9029	8490	7764	6918	6121	5306	4489	3768	3116	25
80	9903	9903	9901	9899	9869	9803	9653	9408	9036	8525	7900	7212	6463	5678	4934	4178	34
90	9813	9813	9813	9813	9803	9768	9672	9543	9309	8966	8526	7937	7201	6576	5862	5165	44
100	9679	9679	9679	9679	9676	9665	9613	9524	9400	9160	8842	8432	7911	7363	6677	6014	52
110	9487	9487	9487	9487	9487	9481	9456	9411	9331	9199	8965	8679	8279	7823	7298	6725	60
120	9233	9233	9233	9233	9233	9228	9219	9196	9147	9053	8913	8697	8442	8098	7637	7152	65
130	8894	8894	8894	8894	8894	8892	8883	8872	8846	8800	8710	8564	8367	8087	7741	7334	68
140	8497	8497	8497	8497	8497	8496	8491	8482	8467	8432	8367	8264	8143	7917	7664	7388	69
150	8024	8024	8024	8024	8024	8023	8021	8016	8006	7980	7942	7873	7792	7632	7433	7177	68
160	7537	7537	7537	7537	7537	7535	7534	7532	7526	7505	7482	7436	7365	7254	7098	6905	66
170	7005	7005	7005	7005	7005	7005	7003	7001	6995	6983	6967	6933	6889	6802	6702	6529	63
180	6453	6453	6453	6453	6453	6453	6452	6450	6449	6440	6422	6401	6372	6311	6208	6087	59
190	5883	5883	5883	5883	5883	5883	5882	5882	5880	5873	5862	5850	5829	5785	5714	5618	54
200	5306	5306	5306	5306	5306	5306	5306	5306	5302	5296	5289	5274	5261	5232	5176	5089	50
210	4777	4777	4777	4777	4777	4777	4777	4777	4775	4772	4769	4761	4751	4728	4681	4616	45
220	4300	4300	4300	4300	4301	4300	4300	4300	4297	4295	4294	4287	4272	4253	4214	4173	41
230	3799	3799	3799	3799	3799	3799	3799	3799	3798	3797	3795	3787	3779	3762	3734	3698	36
240	3324	3324	3324	3324	3324	3324	3324	3324	3322	3321	3319	3316	3309	3290	3272	3243	31
250	2929	2929	2929	2929	2929	2929	2929	2929	2927	2926	2925	2922	2915	2910	2888	2857	28
260	2532	2532	2532	2532	2532	2532	2532	2532	2532	2531	2529	2528	2524	2516	2498	2483	24
270	2180	2180	2180	2180	2180	2180	2180	2180	2180	2180	2178	2177	2175	2165	2152	2135	21
280	1850	1850	1850	1850	1850	1850	1850	1850	1850	1849	1847	1846	1845	1840	1829	1813	17
290	1612	1612	1612	1612	1612	1612	1612	1612	1612	1612	1611	1611	1610	1607	1601	1587	15
300	1410	1410	1410	1410	1410	1410	1410	1410	1410	1409	1409	1409	1407	1406	1399	1390	13
310	1209	1209	1209	1209	1209	1209	1209	1209	1209	1209	1209	1209	1208	1207	1204	1200	1195	11
320	1048	1048	1048	1048	1048	1048	1048	1048	1048	1048	1048	1048	1047	1046	1042	1039	1034	10
330	924	924	924	924	924	924	924	924	924	924	924	924	924	921	917	911	9
340	787	787	787	787	787	787	787	787	787	787	787	787	787	785	784	777	7
350	662	662	662	662	662	662	662	662	662	662	662	661	660	658	656	654	6
360	569	569	569	569	569	569	569	569	569	569	569	568	568	565	564	564	5
370	480	480	480	480	480	480	480	480	479	479	479	479	478	477	476	474	4
380	417	417	417	417	417	417	417	417	417	417	417	417	414	413	412	409	4
390	360	360	360	360	360	360	360	360	360	360	360	359	359	359	356	356	3
400	311	311	311	311	311	311	311	311	311	311	311	311	311	311	311	307	3
410	266	266	266	266	266	266	266	266	266	266	266	266	265	265	264	262	2
420	228	228	228	228	228	228	228	228	228	228	228	228	227	227	227	225	2
430	198	198	198	198	198	198	198	198	198	198	198	198	198	196	196	195	1
440	166	166	166	166	166	166	166	166	166	166	166	166	166	164	164	163	1
450	133	133	133	133	133	133	133	133	133	133	133	133	133	133	132	131	1
460	124	124	124	124	124	124	124	124	124	124	124	124	124	124	124	123	1
470	109	109	109	109	109	109	109	109	109	109	109	109	109	109	109	109	1
480	89	89	89	89	89	89	89	89	89	89	89	89	89	89	89	88	
490	75	75	75	75	75	75	75	75	75	75	75	75	75	75	75	74	

ENERGY DISTRIBUTIONS

NUMBER OF COLLISIONS	NUMBER OF UNDISSOCIATED MOLECULES WITH ENERGIES GREATER THAN -															
	.00	.01	.02	.03	.04	.05	.06	.07	.08	.09	.10	.11	.12	.13	.14	.15
500	62	62	62	62	62	62	62	62	62	62	62	62	62	62	62	61
510	58	58	58	58	58	58	58	58	58	58	58	58	57	57	57	57
520	47	47	47	47	47	47	47	47	47	47	46	46	46	46	46	45
530	41	41	41	41	41	41	41	41	41	41	41	41	41	40	40	40
540	36	36	36	36	36	36	36	36	36	36	36	36	35	34	34	34
550	29	29	29	29	29	29	29	29	29	29	29	29	28	28	28	28
560	26	26	26	26	26	26	26	26	26	26	25	25	25	25	25	25
570	23	23	23	23	23	23	23	23	23	23	23	23	22	22	22	22
580	22	22	22	22	22	22	22	22	22	22	22	22	21	21	21	21
590	21	21	21	21	21	21	21	21	21	21	21	21	21	20	20	20
600	18	18	18	18	18	18	18	18	18	18	18	18	18	17	17	17
610	14	14	14	14	14	14	14	14	14	14	14	14	14	13	13	13
620	13	13	13	13	13	13	13	13	13	13	13	13	13	12	11	11
630	12	12	12	12	12	12	12	12	12	12	12	12	12	11	11	11
640	11	11	11	11	11	11	11	11	11	11	11	11	11	11	10	10
650	10	10	10	10	10	10	10	10	10	10	10	10	10	10	10	10
660	10	10	10	10	10	10	10	10	10	10	10	10	10	10	10	10
670	9	9	9	9	9	9	9	9	9	9	9	9	9	9	9	9
680	9	9	9	9	9	9	9	9	9	9	9	9	9	9	9	9
690	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6
700	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6
710	5	5	5	5	5	5	5	5	5	5	5	5	5	5	5	5
720	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3
730	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2
740	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
750	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
760	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
770	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
780	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
790	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
800	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

ENERGY DISTRIBUTIONS

NUMBER OF COLLISIONS	NUMBER OF UNDISSOCIATED MOLECULES WITH ENERGIES GREATER THAN -															
	..17	.18	.19	.20	.21	.22	.23	.24	.25	.26	.27	.28	.29	.30	.31	.32
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
10	4	1	1	1	1	1	0	0	0	0	0	0	0	0	0	0
20	35	20	17	15	9	5	3	3	3	1	0	0	0	0	0	0
30	133	99	76	54	38	24	17	12	8	6	3	1	1	1	0	0
40	327	254	192	146	102	80	46	32	29	20	13	10	8	3	2	0
50	698	553	419	316	228	166	111	79	54	37	25	16	11	5	2	0
60	1283	1022	783	588	467	341	263	192	141	102	62	44	23	14	7	0
70	2025	1603	1282	1006	802	611	477	350	260	188	132	90	61	37	18	0
80	2873	2344	1888	1542	1218	942	744	567	418	316	226	162	111	72	32	0
90	3738	3138	2604	2157	1762	1414	1125	852	659	498	378	256	172	107	52	0
100	4599	3944	3329	2777	2340	1941	1575	1239	942	719	534	397	283	166	84	0
110	5406	4727	4066	3443	2964	2473	2019	1615	1272	975	737	526	369	227	102	0
120	5969	5325	4716	4097	3493	2951	2454	2035	1610	1243	949	715	498	322	144	0
130	6307	5723	5140	4538	3951	3369	2831	2348	1922	1510	1174	886	631	401	192	0
140	6477	5949	5405	4826	4240	3655	3090	2589	2156	1742	1418	1020	735	484	238	0
150	6450	6034	5551	4991	4447	3881	3303	2759	2324	1914	1518	1158	829	558	257	0
160	6289	5907	5481	4997	4480	3949	3418	2871	2373	1952	1567	1209	887	588	299	0
170	6067	5720	5302	4894	4406	3958	3447	2915	2468	2028	1607	1252	911	616	299	0
180	5699	5405	5068	4681	4308	3862	3407	2950	2526	2079	1674	1304	971	632	312	0
190	5291	5056	4754	4434	4088	3669	3239	2854	2395	1992	1597	1274	978	652	315	0
200	4851	4656	4399	4113	3816	3460	3095	2707	2320	1909	1549	1206	948	655	296	0
210	4412	4269	4054	3815	3574	3272	2941	2579	2227	1808	1502	1204	906	621	312	0
220	4008	3875	3698	3486	3267	3013	2720	2414	2087	1737	1451	1141	872	621	307	0
230	3566	3457	3315	3152	2934	2709	2461	2183	1918	1624	1320	1067	835	587	316	0
240	3125	3035	2923	2771	2592	2405	2209	1966	1727	1482	1239	985	747	533	281	0
250	2754	2705	2600	2476	2324	2156	1946	1748	1564	1345	1145	944	734	519	257	0
260	2398	2343	2253	2150	2031	1890	1722	1531	1361	1168	995	806	634	443	236	0
270	2081	2027	1967	1877	1772	1637	1492	1331	1157	988	852	663	516	371	203	0
280	1766	1729	1685	1611	1504	1398	1254	1108	962	822	666	538	433	297	156	0
290	1544	1514	1466	1408	1322	1219	1113	994	870	745	612	495	374	253	131	0
300	1349	1323	1288	1229	1166	1087	989	885	765	647	529	439	340	244	141	0
310	1165	1144	1104	1074	1019	950	861	762	663	569	473	388	297	215	121	0
320	1011	998	966	923	875	821	751	680	593	523	430	349	274	185	84	0
330	892	873	852	819	774	714	657	598	538	474	407	332	262	193	92	0
340	760	745	720	698	662	618	561	519	463	407	336	282	220	159	75	0
350	637	618	603	578	556	509	473	418	373	331	269	224	164	114	57	0
360	551	536	524	498	474	436	399	367	320	271	228	194	145	98	57	0
370	463	458	444	429	397	365	338	308	258	222	183	153	124	78	41	0
380	400	397	390	369	346	315	289	260	236	196	160	129	99	74	41	0
390	348	340	331	316	300	280	251	231	206	175	150	119	90	67	31	0
400	298	295	288	279	267	252	233	203	174	147	132	106	85	56	25	0
410	254	254	245	234	219	208	194	172	151	131	105	87	72	50	27	0
420	221	216	211	204	197	186	167	149	127	109	90	75	66	48	24	0
430	188	186	182	179	171	165	147	134	112	98	81	69	55	41	26	0
440	160	157	156	148	143	133	119	110	99	87	73	60	43	34	15	0
450	128	126	124	120	117	112	104	88	77	68	59	42	30	16	5	0
460	121	117	115	114	110	102	93	85	78	58	53	43	30	20	11	0
470	106	106	103	101	98	90	85	74	64	57	51	40	26	19	11	0
480	87	87	83	78	75	72	65	62	57	48	40	29	19	13	9	0
490	73	73	72	65	62	59	58	53	50	44	35	31	22	14	9	0

ENERGY DISTRIBUTIONS

NUMBER OF COLLISIONS	NUMBER OF UNDISSOCIATED MOLECULES WITH ENERGIES GREATER THAN -															
	.17	.18	.19	.20	.21	.22	.23	.24	.25	.26	.27	.28	.29	.30	.31	.32
500	60	60	59	59	53	51	49	47	45	37	34	23	17	9	0	0
510	56	54	52	52	50	48	46	42	41	35	31	25	18	14	0	0
520	45	45	45	41	39	37	36	33	31	28	22	21	18	12	6	0
530	38	38	38	38	34	33	31	30	29	25	21	18	15	8	5	0
540	33	33	32	31	31	28	25	24	23	21	18	16	13	8	2	0
550	27	27	26	26	25	25	20	17	14	13	11	9	8	7	2	0
560	23	23	23	22	22	20	16	15	10	9	8	6	5	5	4	0
570	22	22	21	21	18	18	17	14	10	8	7	5	3	2	1	0
580	20	19	19	19	17	14	13	12	10	5	4	4	4	2	1	0
590	20	19	19	18	18	17	16	14	11	8	6	5	5	5	3	0
600	17	17	17	16	15	14	11	11	9	8	8	7	7	6	2	0
610	12	12	12	11	11	10	8	7	6	5	5	5	4	3	1	0
620	11	11	11	11	11	10	8	7	6	5	4	4	2	2	1	0
630	10	10	10	10	10	9	7	6	6	5	5	5	5	5	1	0
640	9	9	9	9	9	8	7	4	3	2	1	1	1	1	1	0
650	8	8	8	8	8	7	6	6	6	5	2	1	0	0	0	0
660	10	10	9	9	9	8	8	6	5	5	4	4	1	0	0	0
670	9	9	9	9	8	7	7	6	6	5	4	4	4	1	0	0
680	9	9	9	9	9	9	8	6	6	6	5	5	4	3	0	0
690	6	6	6	6	6	6	6	6	4	3	3	3	2	1	0	0
700	6	6	6	6	6	5	5	5	5	5	5	3	3	1	0	0
710	5	5	5	5	5	4	4	4	4	4	3	3	2	2	1	0
720	3	3	3	3	2	2	2	2	2	2	2	2	1	1	1	0
730	2	2	2	2	2	1	1	1	1	1	1	1	1	1	1	0
740	1	1	1	1	1	0	0	0	0	0	0	0	0	0	0	0
750	1	1	1	1	1	1	1	1	0	0	0	0	0	0	0	0
760	1	1	1	1	1	1	1	1	1	0	0	0	0	0	0	0
770	1	1	1	1	1	1	1	1	1	1	0	0	0	0	0	0
780	1	1	1	1	1	1	1	1	1	1	1	1	0	0	0	0
790	1	1	1	1	1	1	1	1	1	1	1	1	1	1	0	0
800	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

APPENDIX F

PROBABILITY DISTRIBUTION: RANDOM NUMBER MAPPINGS

SET 1 MBC = 10.)DE , MBC2 = 0. , T = 1800.

ZH	DELHBC	*	DELHBC RANGE	ZHM	DELMBC2	*	DELMBC2 RANGE	ZM	DELMBC2
******	*******	*	*****	******	*****	*	*****	******	*******
0.	0.		0	0.9493	0		+E-02	0.	0.001
0.7596	0.		0	1.0000	+E-02		+E-02	0.2770	0.002
0.7597	0.0001		+E-03	0.0060	0		+E-02	0.4527	0.003
0.7697	0.0002		+E-03	0.1437	+E-02		+E-02	0.5811	0.004
0.7768	0.0003		+E-03	1.0000	+E-01		+E-02	0.7297	0.005
0.7857	0.0004		+E-02	0.1238	+E-01		+E-02	0.7905	0.006
0.7903	0.0005		+E-02	1.0000	+E 00		+E-02	0.8514	0.007
0.7953	0.0006		+E-01	0.3267	+E 00		+E-02	0.9122	0.008
0.7993	0.0007		+E-01	1.0000	+E+01		+E-02	0.9527	0.009
0.8020	0.0008						+E-02	1.0000	0.010
0.8063	0.0009						+E-01	0.	0.010
0.8110	0.0010						+E-01	0.1856	0.020
0.8430	0.0020						+E-01	0.3505	0.030
0.8630	0.0030						+E-01	0.4897	0.040
0.8787	0.0040						+E-01	0.5670	0.050
0.8944	0.0050						+E-01	0.6443	0.060
0.9033	0.0060						+E-01	0.7474	0.070
0.9116	0.0070						+E-01	0.8351	0.080
0.9221	0.0080						+E-01	0.9278	0.090
0.9304	0.0090						+E-01	1.0000	0.100
0.9378	0.0100						+E 00	0.	0.100
0.9760	0.0200						+E 00	0.2670	0.200
0.9880	0.0300						+E 00	0.4450	0.300
0.9951	0.0400						+E 00	0.5808	0.400
0.9975	0.0500						+E 00	0.6815	0.500
0.9985	0.0600						+E 00	0.7869	0.600
0.9994	0.0700						+E 00	0.8735	0.700
0.9997	0.0800						+E 00	0.9204	0.800
1.0000	0.0900						+E 00	0.9602	0.900
							+E 00	1.0000	1.000
							+E+01	0.	1.000
							+E+01	0.7132	2.000
							+E+01	0.9118	3.000
							+E+01	0.9706	4.000
							+E+01	0.9926	5.000
							+E+01	1.0000	6.000

SET 2 HBC = (0.1000)DE , MBC2 = 0. , T = 1800.

ZH	DELHBC	*	DELHBC RANGE	ZHM	DELMBC2	*	DELMBC2 RANGE	ZM	DELMBC2
******	*******	*	*****	******	*****	*	*****	******	*******
0.	-0.0200		-E-01	1.0000	+E-01		+E-02	0.	0.001
0.0003	-0.0100		-E-02	0.1875	+E-02		+E-02	0.2410	0.002
0.0006	-0.0080		-E-02	0.5625	+E-01		+E-02	0.4277	0.003
0.0010	-0.0040		-E-02	1.0000	+E 00		+E-02	0.5663	0.004
0.0016	-0.0030		-E-03	0.0690	0		+E-02	0.7229	0.005
0.0029	-0.0020		-E-03	0.4828	+E-02		+E-02	0.8373	0.006
0.0054	-0.0010		-E-03	0.8276	+E-01		+E-02	0.8795	0.007
0.0057	-0.0009		-E-03	1.0000	+E 00		+E-02	0.9398	0.008
0.0067	-0.0008		0	0.9396	0		+E-02	0.9699	0.009
0.0079	-0.0007		0	0.9966	+E-02		+E-02	1.0000	0.010
0.0083	-0.0006		0	0.9992	+E-01		+E-01	0.	0.010
0.0092	-0.0005		0	1.0000	+E 00		+E-01	0.2412	0.020
0.0111	-0.0004		+E-03	0.0062	0		+E-01	0.4121	0.030
0.0124	-0.0003		+E-03	0.0938	+E-02		+E-01	0.5226	0.040
0.0127	-0.0002		+E-03	0.9312	+E-01		+E-01	0.6181	0.050
0.0146	-0.0001		+E-03	1.0000	+E 00		+E-01	0.6784	0.060
0.0147	0.		+E-02	0.0028	+E-02		+E-01	0.7839	0.070
0.7728	0.		+E-02	0.1194	+E-01		+E-01	0.8492	0.080
0.7729	0.0001		+E-02	0.9750	+E 00		+E-01	0.9347	0.090
0.7823	0.0002		+E-02	1.0000	+E+01		+E-01	1.0000	0.100
0.7915	0.0003		+E-01	0.3057	+E 00		+E 00	0.	0.100
0.7995	0.0004		+E-01	1.0000	+E+01		+E 00	0.2806	0.200
0.8036	0.0005		+E 00	1.0000	+E+01		+E 00	0.4566	0.300
0.8068	0.0006						+E 00	0.5689	0.400
0.8106	0.0007						+E 00	0.6429	0.500
0.8138	0.0008						+E 00	0.7551	0.600
0.8186	0.0009						+E 00	0.8469	0.700
0.8236	0.0010						+E 00	0.9158	0.800
0.8503	0.0020						+E 00	0.9566	0.900
0.8704	0.0030						+E 00	1.0000	1.000
0.8853	0.0040						+E+01	0.	1.000
0.8964	0.0050						+E+01	0.7379	2.000
0.9040	0.0060						+E+01	0.9103	3.000
0.9145	0.0070						+E+01	0.9724	4.000
0.9228	0.0080						+E+01	0.9931	5.000
0.9314	0.0090						+E+01	1.0000	6.000
0.9380	0.0100								
0.9739	0.0200								
0.9882	0.0300								
0.9956	0.0400								
0.9984	0.0500								
0.9987	0.0600								
0.9994	0.0700								
1.0000	0.2000								

SET 3 HBC = (0.1000)DE , MBC2 = 0.01 , T = 1800.

ZH	DELHBC	*	DELHBC RANGE	ZHM	DELMBC2	*	DELMBC2 RANGE	ZM	DELMBC2
******	*******	*	*****	******	*****	*	*****	******	*******
0.	-0.0100		-E-01	1.0000	+E-01		-E-02	0.	-0.010
0.0003	-0.0090		-E-02	0.0435	-E-02		-E-02	0.0635	-0.009
0.0006	-0.0060		-E-02	0.1304	0		-E-02	0.1190	-0.008
0.0009	-0.0050		-E-02	0.1739	+E-02		-E-02	0.2063	-0.007
0.0013	-0.0040		-E-02	0.5652	+E-01		-E-02	0.3254	-0.006
0.0035	-0.0030		-E-02	0.9565	+E 00		-E-02	0.3968	-0.005
0.0044	-0.0020		-E-02	1.0000	+E+01		-E-02	0.5079	-0.004
0.0076	-0.0010		-E-03	0.6377	-E-02		-E-02	0.6270	-0.003
0.0079	-0.0007		-E-03	0.7101	0		-E-02	0.7778	-0.002
0.0088	-0.0006		-E-03	0.8116	+E-02		-E-02	1.0000	-0.001
0.0104	-0.0005		-E-03	0.9420	+E-01		+E-02	0.	0.001
0.0107	-0.0004		-E-03	0.9710	+E 00		+E-02	0.2150	0.002
0.0113	-0.0003		-E-03	1.0000	+E+01		+E-02	0.3271	0.003
0.0129	-0.0002		0	0.0302	-E-02		+E-02	0.4579	0.004
0.0280	-0.0001		0	0.9656	0		+E-02	0.5607	0.005
0.0281	0.		0	0.9970	+E-02		+E-02	0.6355	0.006
0.7704	0.		0	1.0000	+E+01		+E-02	0.7103	0.007
0.7705	0.0001		+E-03	0.0422	-E-02		+E-02	0.7664	0.008
0.7883	0.0002		+E-03	0.1988	+E-02		+E-02	0.8785	0.009
0.7968	0.0003		+E-03	0.9337	+E-01		+E-02	1.0000	0.010
0.8038	0.0004		+E-03	1.0000	+E 00		+E-01	0.	0.010
0.8091	0.0005		+E-02	0.0054	-E-02		+E-01	0.2718	0.020
0.8121	0.0006		+E-02	0.0081	+E-02		+E-01	0.4308	0.030
0.8167	0.0007		+E-02	0.1297	+E-01		+E-01	0.5897	0.040
0.8198	0.0008		+E-02	0.9892	+E 00		+E-01	0.6769	0.050
0.8214	0.0009		+E-02	1.0000	+E+01		+E-01	0.7436	0.060
0.8227	0.0010		+E-01	0.3125	+E 00		+E-01	0.8103	0.070
0.8491	0.0020		+E-01	1.0000	+E+01		+E-01	0.8821	0.080
0.8683	0.0030						+E-01	0.9744	0.090
0.8825	0.0040						+E-01	1.0000	0.100
0.8964	0.0050						+E 00	0.	0.100
0.9071	0.0060						+E 00	0.2180	0.200
0.9181	0.0070						+E 00	0.3910	0.300
0.9298	0.0080						+E 00	0.5263	0.400
0.9348	0.0090						+E 00	0.6742	0.500
0.9402	0.0100						+E 00	0.7794	0.600
0.9735	0.0200						+E 00	0.8571	0.700
0.9880	0.0300						+E 00	0.8947	0.800
0.9956	0.0400						+E 00	0.9599	0.900
0.9975	0.0500						+E 00	1.0000	1.000
0.9984	0.0600						+E+01	0.	1.000
0.9991	0.0700						+E+01	0.7194	2.000
0.9994	0.0800						+E+01	0.8993	3.000
1.0000	1.0000						+E+01	0.9640	4.000
							+E+01	0.9784	5.000
							+E+01	1.0000	6.000

SET 4 HBC = (0.1000)DE , MBC2 = 0.10 , T = 1800.

ZH	DELHBC	*	DELHBC RANGE	ZHM	DELMBC2	*	DELMBC2 RANGE	ZM	DELMBC2
******	*******	*	*****	******	*****	*	*****	******	*******
0.	-0.0200		-E-01	0.5000	+E-01		-E-01	0.	-0.100
0.0006	-0.0100		-E-01	1.0000	+E 00		-E-01	0.0842	-0.090
0.0013	-0.0080		-E-02	0.6351	-E-01		-E-01	0.1632	-0.080
0.0025	-0.0070		-E-02	0.6622	-E-02		-E-01	0.2105	-0.070
0.0035	-0.0060		-E-02	0.7027	+E-02		-E-01	0.2947	-0.060
0.0044	-0.0050		-E-02	0.8514	+E-01		-E-01	0.3895	-0.050
0.0054	-0.0040		-E-02	1.0000	+E 00		-E-01	0.4789	-0.040
0.0076	-0.0030		-E-03	0.7616	-E-01		-E-01	0.5842	-0.030
0.0110	-0.0020		-E-03	0.8953	-E-02		-E-01	0.7211	-0.020
0.0240	-0.0010		-E-03	0.9012	0		-E-01	1.0000	-0.010
0.0274	-0.0009		-E-03	0.9128	+E-02		-E-02	0.	-0.010
0.0322	-0.0008		-E-03	0.9767	+E-01		-E-02	0.0769	-0.009
0.0344	-0.0007		-E-03	1.0000	+E 00		-E-02	0.2115	-0.008
0.0394	-0.0006		0	0.0018	-E-01		-E-02	0.3077	-0.007
0.0438	-0.0005		0	0.0128	-E-02		-E-02	0.4038	-0.006
0.0502	-0.0004		0	0.9792	0		-E-02	0.5385	-0.005
0.0546	-0.0003		0	0.9982	+E-02		-E-02	0.6731	-0.004
0.0662	-0.0002		0	0.9991	+E-01		-E-02	0.7692	-0.003
0.0782	-0.0001		0	1.0000	+E 00		-E-02	0.9038	-0.002
0.0783	0.		+E-03	0.0294	-E-01		-E-02	1.0000	-0.001
0.7902	0.		+E-03	0.1029	+E-02		+E-02	0.	0.001
0.7903	0.0001		+E-03	0.9412	+E-01		+E-02	0.1017	0.002
0.8006	0.0002		+E-03	1.0000	+E 00		+E-02	0.2203	0.003
0.8079	0.0003		+E-02	0.0091	-E-01		+E-02	0.3729	0.004
0.8136	0.0004		+E-02	0.0151	-E-02		+E-02	0.5424	0.005
0.8186	0.0005		+E-02	0.0181	+E-02		+E-02	0.6102	0.006
0.8237	0.0006		+E-02	0.1239	+E-01		+E-02	0.6610	0.007
0.8262	0.0007		+E-02	0.9819	+E 00		+E-02	0.7797	0.008
0.8284	0.0008		+E-02	1.0000	+E+01		+E-02	0.8305	0.009
0.8312	0.0009		+E-01	0.0051	-E-01		+E-02	1.0000	0.010
0.8331	0.0010		+E-01	0.4010	+E 00		+E-01	0.	0.010
0.8533	0.0020		+E-01	1.0000	+E+01		+E-01	0.2299	0.020
0.8691	0.0030		+E 00	1.0000	+E+01		+E-01	0.4425	0.030
0.8823	0.0040						+E-01	0.5747	0.040
0.8953	0.0050						+E-01	0.6552	0.050
0.9066	0.0060						+E-01	0.7184	0.060
0.9142	0.0070						+E-01	0.7931	0.070
0.9227	0.0080						+E-01	0.8506	0.080
0.9303	0.0090						+E-01	0.8966	0.090
0.9375	0.0100						+E-01	1.0000	0.100
0.9732	0.0200						+E 00	0.	0.100
0.9886	0.0300						+E 00	0.2036	0.200
0.9950	0.0400						+E 00	0.3608	0.300
0.9975	0.0500						+E 00	0.4948	0.400
0.9981	0.0600						+E 00	0.6314	0.500
0.9991	0.0700						+E 00	0.7062	0.600
0.9994	0.0800						+E 00	0.7964	0.700
0.9997	0.0900						+E 00	0.8582	0.800
1.0000	0.2000						+E 00	0.9098	0.900
							+E 00	1.0000	1.000
							+E+01	0.	1.000
							+E+01	0.6480	2.000
							+E+01	0.8880	3.000
							+E+01	0.9680	4.000
							+E+01	0.9840	5.000
							+E+01	0.9920	6.000
							+E+01	1.0000	7.000

SET 7 HBC = (0.5000)DE , MBC2 = 0. , T = 1800.

ZH	DELHBC	*	DELHBC RANGE	ZHM	DELMBC2	*	DELMBC2 RANGE	ZM	DELMBC2
******	*******	*	*****	******	*****	*	*****	******	*******
0.	-0.0800		-E-01	0.0169	0		+E-02	0.	0.001
0.0002	-0.0700		-E-01	0.0339	+E-02		+E-02	0.2574	0.002
0.0004	-0.0600		-E-01	0.1186	+E-01		+E-02	0.4438	0.003
0.0012	-0.0400		-E-01	0.5593	+E 00		+E-02	0.5888	0.004
0.0017	-0.0300		-E-01	1.0000	+E+01		+E-02	0.6953	0.005
0.0057	-0.0200		-E-02	0.0159	0		+E-02	0.8166	0.006
0.0113	-0.0100		-E-02	0.0556	+E-02		+E-02	0.8817	0.007
0.0115	-0.0090		-E-02	0.3016	+E-01		+E-02	0.9379	0.008
0.0136	-0.0080		-E-02	0.8333	+E 00		+E-02	0.9763	0.009
0.0161	-0.0070		-E-02	1.0000	+E+01		+E-02	1.0000	0.010
0.0172	-0.0060		-E-03	0.1910	0		+E-01	0.	0.010
0.0186	-0.0050		-E-03	0.4494	+E-02		+E-01	0.2613	0.020
0.0218	-0.0040		-E-03	0.7978	+E-01		+E-01	0.3677	0.030
0.0254	-0.0030		-E-03	0.9775	+E 00		+E-01	0.4871	0.040
0.0291	-0.0020		-E-03	1.0000	+E+01		+E-01	0.6226	0.050
0.0354	-0.0010		0	0.9275	0		+E-01	0.6935	0.060
0.0360	-0.0009		0	0.9925	+E-02		+E-01	0.7613	0.070
0.0369	-0.0008		0	0.9974	+E-01		+E-01	0.8613	0.080
0.0388	-0.0007		0	0.9997	+E 00		+E-01	0.9387	0.090
0.0394	-0.0006		0	1.0000	+E+01		+E-01	1.0000	0.100
0.0405	-0.0005		+E-03	0.0388	0		+E 00	0.	0.100
0.0413	-0.0004		+E-03	0.2198	+E-02		+E 00	0.2250	0.200
0.0432	-0.0003		+E-03	0.8319	+E-01		+E 00	0.3938	0.300
0.0461	-0.0002		+E-03	0.9828	+E 00		+E 00	0.5375	0.400
0.0524	-0.0001		+E-03	1.0000	+E+01		+E 00	0.6531	0.500
0.0525	0.		+E-02	0.0019	0		+E 00	0.7375	0.600
0.7959	0.		+E-02	0.0263	+E-02		+E 00	0.8094	0.700
0.7960	0.0001		+E-02	0.1707	+E-01		+E 00	0.8859	0.800
0.8097	0.0002		+E-02	0.9099	+E 00		+E 00	0.9438	0.900
0.8147	0.0003		+E-02	1.0000	+E+01		+E 00	1.0000	1.000
0.8197	0.0004		+E-01	0.0033	+E-02		+E+01	0.	1.000
0.8241	0.0005		+E-01	0.0199	+E-01		+E+01	0.6361	2.000
0.8271	0.0006		+E-01	0.3278	+E 00		+E+01	0.8066	3.000
0.8306	0.0007		+E-01	1.0000	+E+01		+E+01	0.8984	4.000
0.8334	0.0008						+E+01	0.9639	5.000
0.8376	0.0009						+E+01	0.9902	6.000
0.8403	0.0010						+E+01	0.9967	7.000
0.8640	0.0020						+E+01	1.0000	8.000
0.8810	0.0030								
0.8948	0.0040								
0.9063	0.0050								
0.9164	0.0060								
0.9227	0.0070								
0.9304	0.0080								
0.9361	0.0090								
0.9422	0.0100								
0.9725	0.0200								
0.9853	0.0300								
0.9920	0.0400								
0.9967	0.0500								
0.9983	0.0600								
0.9989	0.0700								
0.9992	0.0800								
0.9994	0.0900								
1.0000	0.1000								

SET 8 HBC = (0.5000)DE , MBC2 = 0.01 , T = 1800.

ZH	DELHBC	*	DELHBC	ZHM	DELMBC2	*	DELMBC2	ZM	DELMBC2
		*	RANGE		RANGE	*	RANGE		
******	*******	*	*****	******	*****	*	*****	******	*******
0.	-0.0900		-E-01	0.0233	+E-02		-E-02	0.	-0.010
0.0003	-0.0800		-E-01	0.0930	+E-01		-E-02	0.0813	-0.009
0.0007	-0.0400		-E-01	0.5116	+E 00		-E-02	0.1382	-0.008
0.0024	-0.0300		-E-01	1.0000	+E+01		-E-02	0.2276	-0.007
0.0055	-0.0200		-E-02	0.0290	-E-02		-E-02	0.3415	-0.006
0.0148	-0.0100		-E-02	0.0870	0		-E-02	0.4634	-0.005
0.0155	-0.0090		-E-02	0.1449	+E-02		-E-02	0.5691	-0.004
0.0162	-0.0080		-E-02	0.4783	+E-01		-E-02	0.6748	-0.003
0.0186	-0.0070		-E-02	0.9130	+E 00		-E-02	0.8455	-0.002
0.0196	-0.0060		-E-02	1.0000	+E+01		-E-02	1.0000	-0.001
0.0213	-0.0050		-E-03	0.4744	-E-02		+E-02	0.	0.001
0.0237	-0.0040		-E-03	0.5128	0		+E-02	0.1944	0.002
0.0261	-0.0030		-E-03	0.6282	+E-02		+E-02	0.2778	0.003
0.0309	-0.0020		-E-03	0.8333	+E-01		+E-02	0.4074	0.004
0.0385	-0.0010		-E-03	1.0000	+E 00		+E-02	0.5093	0.005
0.0392	-0.0009		0	0.0348	-E-02		+E-02	0.6389	0.006
0.0399	-0.0008		0	0.9585	0		+E-02	0.7407	0.007
0.0409	-0.0007		0	0.9914	+E-02		+E-02	0.8426	0.008
0.0433	-0.0006		0	0.9986	+E-01		+E-02	0.8889	0.009
0.0443	-0.0005		0	1.0000	+E 00		+E-02	1.0000	0.010
0.0457	-0.0004		+E-03	0.0526	-E-02		+E-01	0.	0.010
0.0498	-0.0003		+E-03	0.0658	0		+E-01	0.3368	0.020
0.0526	-0.0002		+E-03	0.2171	+E-02		+E-01	0.4870	0.030
0.0653	-0.0001		+E-03	0.8553	+E-01		+E-01	0.6166	0.040
0.0654	0.		+E-03	0.9868	+E 00		+E-01	0.6943	0.050
0.7856	0.		+E-03	1.0000	+E+01		+E-01	0.7876	0.060
0.7857	0.0001		+E-02	0.0099	-E-02		+E-01	0.8601	0.070
0.8014	0.0002		+E-02	0.0132	0		+E-01	0.9275	0.080
0.8120	0.0003		+E-02	0.0197	+E-02		+E-01	0.9689	0.090
0.8179	0.0004		+E-02	0.1382	+E-01		+E-01	1.0000	0.100
0.8220	0.0005		+E-02	0.9276	+E 00		+E 00	0.	0.100
0.8247	0.0006		+E-02	1.0000	+E+01		+E 00	0.2207	0.200
0.8309	0.0007		+E-01	0.0179	+E-01		+E 00	0.3856	0.300
0.8337	0.0008		+E-01	0.3274	+E 00		+E 00	0.5239	0.400
0.8354	0.0009		+E-01	1.0000	+E+01		+E 00	0.6303	0.500
0.8378	0.0010						+E 00	0.7074	0.600
0.8619	0.0020						+E 00	0.7979	0.700
0.8790	0.0030						+E 00	0.8803	0.800
0.8928	0.0040						+E 00	0.9521	0.900
0.9031	0.0050						+E 00	1.0000	1.000
0.9117	0.0060						+E+01	0.	1.000
0.9182	0.0070						+E+01	0.6098	2.000
0.9258	0.0080						+E+01	0.8232	3.000
0.9344	0.0090						+E+01	0.9085	4.000
0.9423	0.0100						+E+01	0.9695	5.000
0.9732	0.0200						+E+01	0.9878	6.000
0.9863	0.0300						+E+01	0.9939	7.000
0.9938	0.0400						+E+01	1.0000	8.000
0.9972	0.0500								
0.9979	0.0600								
0.9990	0.0700								
0.9997	0.0800								
1.0000	0.1000								

SET 9 HBC = (0.5000)DE , MBC2 = 0.10 , T = 1800.

ZH	DELHBC	*	DELHBC RANGE	ZHM	DELMBC2	*	DELMBC2 RANGE	ZM	DELMBC2
******	*******	*	*****	******	*****	*	*****	******	*******
0.	-0.0700		-E-01	0.0952	-E-01		-E-01	0.	-0.100
0.0003	-0.0600		-E-01	0.1190	-E-02		-E-01	0.0729	-0.090
0.0010	-0.0500		-E-01	0.2619	+E-01		-E-01	0.1250	-0.080
0.0017	-0.0400		-E-01	0.5952	+E 00		-E-01	0.1979	-0.070
0.0038	-0.0300		-E-01	1.0000	+E+01		-E-01	0.2604	-0.060
0.0069	-0.0200		-E-02	0.4667	-E-01		-E-01	0.3073	-0.050
0.0144	-0.0100		-E-02	0.4857	-E-02		-E-01	0.4688	-0.040
0.0151	-0.0090		-E-02	0.4952	+E-02		-E-01	0.5521	-0.030
0.0165	-0.0080		-E-02	0.6762	+E-01		-E-01	0.7500	-0.020
0.0189	-0.0070		-E-02	0.9333	+E 00		-E-01	1.0000	-0.010
0.0213	-0.0060		-E-02	1.0000	+E+01		-E-02	0.	-0.010
0.0240	-0.0050		-E-03	0.7297	-E-01		-E-02	0.1094	-0.009
0.0264	-0.0040		-E-03	0.8446	-E-02		-E-02	0.1406	-0.008
0.0306	-0.0030		-E-03	0.8581	+E-02		-E-02	0.3438	-0.007
0.0374	-0.0020		-E-03	0.9324	+E-01		-E-02	0.4688	-0.006
0.0505	-0.0010		-E-03	0.9932	+E 00		-E-02	0.6094	-0.005
0.0543	-0.0009		-E-03	1.0000	+E+01		-E-02	0.6719	-0.004
0.0563	-0.0008		0	0.0055	-E-01		-E-02	0.7812	-0.003
0.0594	-0.0007		0	0.0228	-E-02		-E-02	0.8594	-0.002
0.0632	-0.0006		0	0.9786	0		-E-02	1.0000	-0.001
0.0680	-0.0005		0	0.9926	+E-02		+E-02	0.	0.001
0.0745	-0.0004		0	0.9985	+E-01		+E-02	0.1509	0.002
0.0814	-0.0003		0	1.0000	+E 00		+E-02	0.2453	0.003
0.0883	-0.0002		+E-03	0.0368	-E-01		+E-02	0.4906	0.004
0.1013	-0.0001		+E-03	0.0735	-E-02		+E-02	0.6038	0.005
0.1014	0.		+E-03	0.2132	+E-02		+E-02	0.6226	0.006
0.7929	0.		+E-03	0.9044	+E-01		+E-02	0.6604	0.007
0.7930	0.0001		+E-03	0.9926	+E 00		+E-02	0.8113	0.008
0.8036	0.0002		+E-03	1.0000	+E+01		+E-02	0.9245	0.009
0.8108	0.0003		+E-02	0.0486	-E-01		+E-02	1.0000	0.010
0.8190	0.0004		+E-02	0.0625	-E-02		+E-01	0.	0.010
0.8249	0.0005		+E-02	0.0660	+E-02		+E-01	0.2471	0.020
0.8293	0.0006		+E-02	0.1736	+E-01		+E-01	0.4253	0.030
0.8317	0.0007		+E-02	0.9132	+E 00		+E-01	0.5172	0.040
0.8341	0.0008		+E-02	1.0000	+E+01		+E-01	0.6437	0.050
0.8379	0.0009		+E-01	0.0056	-E-01		+E-01	0.7184	0.060
0.8396	0.0010		+E-01	0.0168	+E-02		+E-01	0.7644	0.070
0.8602	0.0020		+E-01	0.0223	+E-01		+E-01	0.8218	0.080
0.8760	0.0030		+E-01	0.3966	+E 00		+E-01	0.8966	0.090
0.8870	0.0040		+E-01	1.0000	+E+01		+E-01	1.0000	0.100
0.8984	0.0050						+E 00	0.	0.100
0.9087	0.0060						+E 00	0.1826	0.200
0.9176	0.0070						+E 00	0.3362	0.300
0.9234	0.0080						+E 00	0.4609	0.400
0.9310	0.0090						+E 00	0.5971	0.500
0.9385	0.0100						+E 00	0.7043	0.600
0.9732	0.0200						+E 00	0.7652	0.700
0.9873	0.0300						+E 00	0.8667	0.800
0.9942	0.0400						+E 00	0.9478	0.900
0.9976	0.0500						+E 00	1.0000	1.000
0.9986	0.0600						+E+01	0.	1.000
0.9997	0.0700						+E+01	0.5912	2.000
1.0000	0.1000						+E+01	0.7925	3.000
							+E+01	0.9182	4.000
							+E+01	0.9686	5.000
							+E+01	0.9874	6.000
							+E+01	1.0000	7.000

SET 10 HBC = (0.5000)DE , MBC2 = 1.00 , T = 1800.

ZH	DELHBC	*	DELHBC RANGE	ZHM	DELMBC2	*	DELMBC2 RANGE	ZM	DELMBC2
******	*******	*	*****	******	*****	*	*****	******	*******
0.	-0.0700		-E-01	0.8085	-E 00		-E 00	0.	-1.000
0.0010	-0.0600		-E-01	0.8298	-E-01		-E 00	0.0790	-0.900
0.0031	-0.0300		-E-01	0.8723	+E-01		-E 00	0.1753	-0.800
0.0092	-0.0200		-E-01	0.9468	+E 00		-E 00	0.2612	-0.700
0.0320	-0.0100		-E-01	1.0000	+E+01		-E 00	0.3574	-0.600
0.0381	-0.0090		-E-02	0.7811	-E 00		-E 00	0.4536	-0.500
0.0439	-0.0080		-E-02	0.8798	-E-01		-E 00	0.5464	-0.400
0.0483	-0.0070		-E-02	0.9013	+E-01		-E 00	0.6632	-0.300
0.0565	-0.0060		-E-02	0.9828	+E 00		-E 00	0.7869	-0.200
0.0657	-0.0050		-E-02	1.0000	+E+01		-E 00	1.0000	-0.100
0.0766	-0.0040		-E-03	0.0957	-E 00		-E-01	0.	-0.100
0.0844	-0.0030		-E-03	0.7391	-E-01		-E-01	0.0877	-0.090
0.0947	-0.0020		-E-03	0.8696	-E-02		-E-01	0.1491	-0.080
0.1113	-0.0010		-E-03	0.8957	+E-02		-E-01	0.2018	-0.070
0.1141	-0.0009		-E-03	0.9478	+E-01		-E-01	0.2807	-0.060
0.1171	-0.0008		-E-03	0.9913	+E 00		-E-01	0.3684	-0.050
0.1209	-0.0007		-E-03	1.0000	+E+01		-E-01	0.5088	-0.040
0.1236	-0.0006		0	0.0005	-E 00		-E-01	0.6754	-0.030
0.1273	-0.0005		0	0.0025	-E-01		-E-01	0.8509	-0.020
0.1318	-0.0004		0	0.0051	-E-02		-E-01	1.0000	-0.010
0.1386	-0.0003		0	0.9919	0		-E-02	0.	-0.010
0.1444	-0.0002		0	0.9964	+E-02		-E-02	0.3500	-0.009
0.1505	-0.0001		0	0.9995	+E-01		-E-02	0.5500	-0.008
0.1506	0.		0	1.0000	+E 00		-E-02	0.6500	-0.007
0.8195	0.		+E-03	0.0381	-E 00		-E-02	0.7000	-0.006
0.8196	0.0001		+E-03	0.1048	-E-01		-E-02	0.8000	-0.005
0.8247	0.0002		+E-03	0.1429	+E-02		-E-02	0.8500	-0.004
0.8291	0.0003		+E-03	0.8952	+E-01		-E-02	0.9000	-0.003
0.8342	0.0004		+E-03	0.9905	+E 00		-E-02	0.9500	-0.002
0.8396	0.0005		+E-03	1.0000	+E+01		-E-02	1.0000	-0.001
0.8437	0.0006		+E-02	0.0536	-E 00		+E-02	0.	0.001
0.8464	0.0007		+E-02	0.0625	-E-01		+E-02	0.1667	0.002
0.8495	0.0008		+E-02	0.0670	0		+E-02	0.3333	0.003
0.8512	0.0009		+E-02	0.0759	+E-02		+E-02	0.3989	0.004
0.8553	0.0010		+E-02	0.1830	+E-01		+E-02	0.6111	0.006
0.8723	0.0020		+E-02	0.9375	+E 00		+E-02	0.7778	0.007
0.8825	0.0030		+E-02	1.0000	+E+01		+E-02	0.9444	0.008
0.8931	0.0040		+E-01	0.0250	-E 00		+E-02	1.0000	0.010
0.9013	0.0050		+E-01	0.0350	-E-01		+E-01	0.	0.010
0.9088	0.0060		+E-01	0.0600	+E-01		+E-01	0.1705	0.020
0.9145	0.0070		+E-01	0.2600	+E 00		+E-01	0.3411	0.030
0.9203	0.0080		+E-01	1.0000	+E+01		+E-01	0.4961	0.040
0.9278	0.0090		+E 00	1.0000	+E+01		+E-01	0.5736	0.050
0.9316	0.0100						+E-01	0.6512	0.060
0.9666	0.0200						+E-01	0.7364	0.070
0.9843	0.0300						+E-01	0.8217	0.080
0.9928	0.0400						+E-01	0.9147	0.090
0.9963	0.0500						+E-01	1.0000	0.100
0.9986	0.0600						+E 00	0.	0.100
0.9993	0.0700						+E 00	0.2231	0.200
0.9997	0.0800						+E 00	0.3586	0.300
1.0000	0.2000						+E 00	0.4462	0.400
							+E 00	0.6016	0.500
							+E 00	0.7092	0.600
							+E 00	0.8048	0.700
							+E 00	0.8566	0.800
							+E 00	0.9363	0.900
							+E 00	1.0000	1.000
							+E+01	0.	1.000
							+E+01	0.5287	2.000
							+E+01	0.7529	3.000
							+E+01	0.8793	4.000
							+E+01	0.9483	5.000
							+E+01	0.9655	6.000
							+E+01	0.9943	7.000
							+E+01	1.0000	10.000

SET 11 HBC = (0.50001DE , MBC2 = 1.48 , T = 1800.

ZH	DELHBC	*	DELHBC RANGE	ZHM	DELMBC2	*	DELMBC2 RANGE	ZM	DELMBC2
******	*******	*	*****	******	*****	*	*****	******	*******
0.	-0.0800		-E-01	0.4780	-E+01		-E+01	0.	-1.480
0.0003	-0.0700		-E-01	0.8491	-E 00		-E+01	1.0000	-1.000
0.0006	-0.0600		-E-01	0.8616	-E-01		-E 00	0.	-1.000
0.0015	-0.0500		-E-01	0.8805	+E-01		-E 00	0.0774	-0.900
0.0031	-0.0400		-E-01	0.9623	+E 00		-E 00	0.1481	-0.800
0.0080	-0.0300		-E-01	1.0000	+E+01		-E 00	0.2694	-0.700
0.0173	-0.0200		-E-02	0.0652	-E+01		-E 00	0.3401	-0.600
0.0491	-0.0100		-E-02	0.7971	-E 00		-E 00	0.4276	-0.500
0.0556	-0.0090		-E-02	0.8696	-E-01		-E 00	0.5354	-0.400
0.0611	-0.0080		-E-02	0.8732	0		-E 00	0.6498	-0.300
0.0694	-0.0070		-E-02	0.8804	+E-02		-E 00	0.7811	-0.200
0.0778	-0.0060		-E-02	0.9239	+E-01		-E 00	1.0000	-0.100
0.0864	-0.0050		-E-02	0.9855	+E 00		-E-01	0.	-0.100
0.0938	-0.0040		-E-02	1.0000	+E+01		-E-01	0.0690	-0.090
0.1031	-0.0030		-E-03	0.0388	-E 00		-E-01	0.1552	-0.080
0.1136	-0.0020		-E-03	0.8058	-E-01		-E-01	0.2414	-0.070
0.1343	-0.0010		-E-03	0.8738	-E-02		-E-01	0.3707	-0.060
0.1361	-0.0009		-E-03	0.8835	0		-E-01	0.4224	-0.050
0.1389	-0.0008		-E-03	0.9029	+E-02		-E-01	0.5517	-0.040
0.1414	-0.0007		-E-03	0.9612	+E-01		-E-01	0.7155	-0.030
0.1435	-0.0006		-E-03	1.0000	+E 00		-E-01	0.8448	-0.020
0.1478	-0.0005		0	0.0023	-E-01		-E-01	1.0000	-0.010
0.1528	-0.0004		0	0.0065	-E-02		-E-02	0.	-0.010
0.1559	-0.0003		0	0.9908	0		-E-02	0.2000	-0.009
0.1599	-0.0002		0	0.9972	+E-02		-E-02	0.2500	-0.008
0.1660	-0.0001		0	0.9995	+E-01		-E-02	0.5500	-0.006
0.1661	0.		0	1.0000	+E 00		-E-02	0.7000	-0.004
0.8355	0.		+E-03	0.0202	-E+01		-E-02	0.8000	-0.003
0.8356	0.0001		+E-03	0.1010	-E 00		-E-02	0.9500	-0.002
0.8414	0.0002		+E-03	0.1313	-E-01		-E-02	1.0000	-0.001
0.8454	0.0003		+E-03	0.1616	-E-02		+E-02	0.	0.001
0.8506	0.0004		+E-03	0.1717	+E-02		+E-02	0.1429	0.002
0.8531	0.0005		+E-03	0.9091	+E-01		+E-02	0.2381	0.003
0.8556	0.0006		+E-03	0.9798	+E 00		+E-02	0.4286	0.004
0.8599	0.0007		+E-03	1.0000	+E+01		+E-02	0.5714	0.005
0.8617	0.0008		+E-02	0.0216	-E+01		+E-02	0.6190	0.006
0.8645	0.0009		+E-02	0.0996	-E 00		+E-02	0.7143	0.007
0.8660	0.0010		+E-02	0.1155	-E-01		+E-02	0.9524	0.008
0.8827	0.0020		+E-02	0.1299	-E-02		+E-02	1.0000	0.010
0.8954	0.0030		+E-02	0.1385	+E-02		+E-01	0.	0.010
0.9059	0.0040		+E-02	0.2121	+E-01		+E-01	0.1897	0.020
0.9108	0.0050		+E-02	0.9177	+E 00		+E-01	0.3190	0.030
0.9185	0.0060		+E-02	1.0000	+E+01		+E-01	0.4483	0.040
0.9250	0.0070		+E-01	0.0050	-E+01		+E-01	0.5517	0.050
0.9299	0.0080		+E-01	0.0347	-E 00		+E-01	0.6638	0.060
0.9343	0.0090		+E-01	0.0396	-E-01		+E-01	0.7672	0.070
0.9373	0.0100		+E-01	0.2426	+E 00		+E-01	0.8621	0.080
0.9654	0.0200		+E-01	1.0000	+E+01		+E-01	0.9224	0.090
0.9852	0.0300		+E 00	1.0000	+E+01		+E-01	1.0000	0.100
0.9917	0.0400						+E 00	0.	0.100
0.9944	0.0500						+E 00	0.2683	0.200
0.9966	0.0600						+E 00	0.4309	0.300
0.9981	0.0700						+E 00	0.5244	0.400
0.9991	0.0800						+E 00	0.6057	0.500
0.9994	0.0900						+E 00	0.7073	0.600
0.9997	0.1000						+E 00	0.8089	0.700
1.0000	0.2000						+E 00	0.8699	0.800
							+E 00	0.9472	0.900
							+E 00	1.0000	1.000
							+E+01	0.	1.000
							+E+01	0.5189	2.000
							+E+01	0.7297	3.000
							+E+01	0.8703	4.000
							+E+01	0.9189	5.000
							+E+01	0.9514	6.000
							+E+01	0.9730	7.000
							+E+01	0.9892	8.000
							+E+01	1.0000	9.000

SET 12 HBC = (0.5000)DE , MBC2 = 2.00 , T = 1800.

ZH	DELHBC	*	DELHBC RANGE	ZHM	DELMBC2	*	DELMBC2 RANGE	ZM	DELMBC2
******	*******	*	*****	******	*****	*	*****	******	*******
0.	-0.0800		-E-01	0.6146	-E+01		-E+01	0.	-2.000
0.0003	-0.0700		-E-01	0.9062	-E 00		-E+01	1.0000	-1.000
0.0017	-0.0600		-E-01	0.9167	-E-01		-E 00	0.	-1.000
0.0030	-0.0500		-E-01	0.9219	+E-02		-E 00	0.0620	-0.900
0.0061	-0.0400		-E-01	0.9323	+E-01		-E 00	0.1512	-0.800
0.0108	-0.0300		-E-01	0.9896	+E 00		-E 00	0.2442	-0.700
0.0270	-0.0200		-E-01	1.0000	+E+01		-E 00	0.3101	-0.600
0.0647	-0.0100		-E-02	0.0797	-E+01		-E 00	0.4147	-0.500
0.0711	-0.0090		-E-02	0.7769	-E 00		-E 00	0.5388	-0.400
0.0772	-0.0080		-E-02	0.8725	-E-01		-E 00	0.6589	-0.300
0.0836	-0.0070		-E-02	0.8765	-E-02		-E 00	0.7868	-0.200
0.0920	-0.0060		-E-02	0.9084	+E-01		-E 00	1.0000	-0.100
0.1014	-0.0050		-E-02	0.9920	+E 00		-E-01	0.	-0.100
0.1095	-0.0040		-E-02	1.0000	+E+01		-E-01	0.1121	-0.090
0.1179	-0.0030		-E-03	0.0761	-E 00		-E-01	0.1869	-0.080
0.1311	-0.0020		-E-03	0.8370	-E-01		-E-01	0.3084	-0.070
0.1493	-0.0010		-E-03	0.8804	-E-02		-E-01	0.3832	-0.060
0.1516	-0.0009		-E-03	0.9130	+E-02		-E-01	0.4579	-0.050
0.1546	-0.0008		-E-03	0.9457	+E-01		-E-01	0.5794	-0.040
0.1563	-0.0007		-E-03	0.9891	+E 00		-E-01	0.6729	-0.030
0.1594	-0.0006		-E-03	1.0000	+E+01		-E-01	0.8318	-0.020
0.1624	-0.0005		0	0.0005	-E 00		-E-01	1.0000	-0.010
0.1664	-0.0004		0	0.0015	-E-01		-E-02	0.	-0.010
0.1715	-0.0003		0	0.0050	-E-02		-E-02	0.1667	-0.009
0.1745	-0.0002		0	0.9945	0		-E-02	0.2500	-0.008
0.1803	-0.0001		0	0.9980	+E-02		-E-02	0.3333	-0.007
0.1804	0.		0	0.9995	+E-01		-E-02	0.4167	-0.006
0.8518	0.		0	1.0000	+E 00		-E-02	0.5000	-0.005
0.8519	0.0001		+E-03	0.0132	-E+01		-E-02	0.5833	-0.004
0.8558	0.0002		+E-03	0.0263	-E 00		-E-02	0.6667	-0.003
0.8608	0.0003		+E-03	0.0658	-E-01		-E-02	0.7500	-0.002
0.8632	0.0004		+E-03	0.1053	+E-02		-E-02	1.0000	-0.001
0.8659	0.0005		+E-03	0.9079	+E-01		+E-02	0.	0.001
0.8689	0.0006		+E-03	0.9868	+E 00		+E-02	0.0714	0.002
0.8716	0.0007		+E-03	1.0000	+E+01		+E-02	0.2143	0.003
0.8730	0.0008		+E-02	0.0106	-E+01		+E-02	0.4286	0.004
0.8760	0.0009		+E-02	0.0688	-E 00		+E-02	0.5714	0.006
0.8774	0.0010		+E-02	0.0899	-E-01		+E-02	0.6429	0.007
0.8952	0.0020		+E-02	0.2011	+E-01		+E-02	0.7143	0.008
0.9043	0.0030		+E-02	0.9312	+E 00		+E-02	0.9286	0.009
0.9111	0.0040		+E-02	1.0000	+E+01		+E-02	1.0000	0.010
0.9161	0.0050		+E-01	0.0057	-E+01		+E-01	0.	0.010
0.9212	0.0060		+E-01	0.0460	-E 00		+E-01	0.1616	0.020
0.9276	0.0070		+E-01	0.0575	-E-01		+E-01	0.2929	0.030
0.9336	0.0080		+E-01	0.0632	+E-01		+E-01	0.3939	0.040
0.9377	0.0090		+E-01	0.2586	+E 00		+E-01	0.5152	0.050
0.9410	0.0100		+E-01	1.0000	+E+01		+E-01	0.6162	0.060
0.9697	0.0200		+E 00	1.0000	+E+01		+E-01	0.6869	0.070
0.9825	0.0300						+E-01	0.7980	0.080
0.9902	0.0400						+E-01	0.9091	0.090
0.9933	0.0500						+E-01	1.0000	0.100
0.9960	0.0600						+E 00	0.	0.100
0.9973	0.0700						+E 00	0.2558	0.200
0.9980	0.0800						+E 00	0.3860	0.300
0.9990	0.0900						+E 00	0.5256	0.400
0.9997	0.1000						+E 00	0.6140	0.500
1.0000	0.2000						+E 00	0.7163	0.600
							+E 00	0.8000	0.700
							+E 00	0.8651	0.800
							+E 00	0.9349	0.900
							+E 00	1.0000	1.000
							+E+01	0.	1.000
							+E+01	0.5168	2.000
							+E+01	0.7248	3.000
							+E+01	0.8456	4.000
							+E+01	0.9060	5.000
							+E+01	0.9463	6.000
							+E+01	0.9597	7.000
							+E+01	0.9799	8.000
							+E+01	1.0000	9.000

SET 13 , HBC = (0.50001)DE , MBC2 = 5.00 , T = 1800.

ZH	DELHBC	*	DELHBC RANGE	ZHM	DELMBC2	*	DELMBC2 RANGE	ZM	DELMBC2
******	*******	*	*****	******	*****	*	*****	******	*******
0.	-0.1596		-E 00	1.0000	-E+01		-E+01	0.	-5.000
0.0007	-0.1000		-E-01	0.8533	-E+01		-E+01	0.1175	-4.000
0.0023	-0.0900		-E-01	0.9701	-E 00		-E+01	0.3494	-3.000
0.0039	-0.0800		-E-01	0.9755	-E-01		-E+01	0.6114	-2.000
0.0075	-0.0700		-E-01	0.9783	+E-01		-E+01	1.0000	-1.000
0.0134	-0.0600		-E-01	1.0000	+E 00		-E 00	0.	-1.000
0.0213	-0.0500		-E-02	0.0647	-E+01		-E 00	0.0546	-0.900
0.0354	-0.0400		-E-02	0.8118	-E 00		-E 00	0.1257	-0.800
0.0560	-0.0300		-E-02	0.9353	-E-01		-E 00	0.2295	-0.700
0.0852	-0.0200		-E-02	0.9471	+E-01		-E 00	0.3388	-0.600
0.1212	-0.0100		-E-02	0.9941	+E 00		-E 00	0.4426	-0.500
0.1271	-0.0090		-E-02	1.0000	+E+01		-E 00	0.5355	-0.400
0.1307	-0.0080		-E-03	0.0441	-E 00		-E 00	0.6721	-0.300
0.1346	-0.0070		-E-03	0.8382	-E-01		-E 00	0.8306	-0.200
0.1402	-0.0060		-E-03	0.8824	-E-02		-E 00	1.0000	-0.100
0.1477	-0.0050		-E-03	0.8971	0		-E-01	0.	-0.100
0.1539	-0.0040		-E-03	0.9265	+E-01		-E-01	0.0778	-0.090
0.1595	-0.0030		-E-03	1.0000	+E 00		-E-01	0.1667	-0.080
0.1677	-0.0020		0	0.0005	-E 00		-E-01	0.2000	-0.070
0.1769	-0.0010		0	0.0024	-E-01		-E-01	0.2778	-0.060
0.1788	-0.0009		0	0.0058	-E-02		-E-01	0.3333	-0.050
0.1795	-0.0008		0	0.9961	0		-E-01	0.4889	-0.040
0.1811	-0.0007		0	0.9986	+E-02		-E-01	0.6778	-0.030
0.1834	-0.0006		0	1.0000	+E-01		-E-01	0.8444	-0.020
0.1851	-0.0005		+E-03	0.0448	-E 00		-E-01	1.0000	-0.010
0.1890	-0.0004		+E-03	0.0896	-E-01		-E-02	0.	-0.010
0.1936	-0.0003		+E-03	0.1194	-E-02		-E-02	0.3333	-0.009
0.1965	-0.0002		+E-03	0.2239	+E-02		-E-02	0.4167	-0.008
0.1991	-0.0001		+E-03	0.8955	+E-01		-E-02	0.6667	-0.007
0.1992	0.		+E-03	1.0000	+E 00		-E-02	0.7500	-0.004
0.8788	0.		+E-02	0.0168	-E+01		-E-02	0.8333	-0.002
0.8789	0.0001		+E-02	0.0335	-E 00		-E-02	1.0000	-0.001
0.8811	0.0002		+E-02	0.0615	-E-01		+E-02	0.	0.002
0.8840	0.0003		+E-02	0.0670	+E-02		+E-02	0.1538	0.003
0.8870	0.0004		+E-02	0.2011	+E-01		+E-02	0.3846	0.004
0.8909	0.0005		+E-02	0.8994	+E 00		+E-02	0.5385	0.006
0.8935	0.0006		+E-02	1.0000	+E+01		+E-02	0.7692	0.007
0.8952	0.0007		+E-01	0.0161	-E+01		+E-02	0.9231	0.008
0.8968	0.0008		+E-01	0.0403	-E 00		+E-02	1.0000	0.010
0.8991	0.0009		+E-01	0.0484	-E-01		+E-01	0.	0.010
0.9008	0.0010		+E-01	0.3145	+E 00		+E-01	0.1818	0.020
0.9142	0.0020		+E-01	1.0000	+E+01		+E-01	0.2857	0.030
0.9250	0.0030						+E-01	0.4416	0.040
0.9325	0.0040						+E-01	0.5195	0.050
0.9371	0.0050						+E-01	0.5844	0.060
0.9417	0.0060						+E-01	0.7013	0.070
0.9456	0.0070						+E-01	0.7792	0.080
0.9502	0.0080						+E-01	0.9091	0.090
0.9548	0.0090						+E-01	1.0000	0.100
0.9594	0.0100						+E 00	0.	0.100
0.9826	0.0200						+E 00	0.2419	0.200
0.9895	0.0300						+E 00	0.4301	0.300
0.9951	0.0400						+E 00	0.5269	0.400
0.9974	0.0500						+E 00	0.6290	0.500
0.9984	0.0600						+E 00	0.7204	0.600
0.9987	0.0700						+E 00	0.8011	0.700
0.9990	0.0800						+E 00	0.9140	0.800
0.9997	0.0900						+E 00	0.9409	0.900
1.0000	0.1000						+E 00	1.0000	1.000
							+E+01	0.	1.000
							+E+01	0.6058	2.000
							+E+01	0.8462	3.000
							+E+01	0.9423	4.000
							+E+01	0.9615	5.000
							+E+01	0.9712	6.000
							+E+01	0.9904	8.000
							+E+01	1.0000	10.000

SET 14 HBC = (0.5000)DE , MBC2 = 10.00 , T = 1800.

ZH	DELHBC	*	DELHBC RANGE	ZHM	DELMBC2	*	DELMBC2 RANGE	ZM	DELMBC2
******	*******	*	*****	******	*****	*	*****	******	*******
0.	-0.1596		-E 00	1.0000	-E+01		-E+01	0.	-10.000
0.0063	-0.1000		-E-01	0.8835	-E+01		-E+01	0.0053	-9.000
0.0094	-0.0900		-E-01	1.0000	-E 00		-E+01	0.0213	-8.000
0.0135	-0.0800		-E-02	0.0316	-E+01		-E+01	0.0613	-7.000
0.0186	-0.0700		-E-02	0.7722	-E 00		-E+01	0.1147	-6.000
0.0296	-0.0600		-E-02	0.9367	-E-01		-E+01	0.1947	-5.000
0.0422	-0.0500		-E-02	0.9430	+E-01		-E+01	0.3360	-4.000
0.0567	-0.0400		-E-02	1.0000	+E 00		-E+01	0.4960	-3.000
0.0752	-0.0300		-E-03	0.1061	-E 00		-E+01	0.7173	-2.000
0.0995	-0.0200		-E-03	0.7879	-E-01		-E+01	1.0000	-1.000
0.1306	-0.0100		-E-03	0.8788	-E-02		-E 00	0.	-1.000
0.1347	-0.0090		-E-03	0.9394	+E-01		-E 00	0.0663	-0.900
0.1379	-0.0080		-E-03	1.0000	+E 00		-E 00	0.1381	-0.800
0.1423	-0.0070		0	0.0009	-E 00		-E 00	0.1878	-0.700
0.1483	-0.0060		0	0.0014	-E-01		-E 00	0.3094	-0.600
0.1517	-0.0050		0	0.0045	-E-02		-E 00	0.4475	-0.500
0.1599	-0.0040		0	0.9927	0		-E 00	0.6077	-0.400
0.1646	-0.0030		0	0.9973	+E-02		-E 00	0.7127	-0.300
0.1709	-0.0020		0	1.0000	+E-01		-E 00	0.8453	-0.200
0.1804	-0.0010		+E-03	0.0690	-E 00		-E 00	1.0000	-0.100
0.1819	-0.0009		+E-03	0.0862	-E-01		-E-01	0.	-0.100
0.1835	-0.0008		+E-03	0.1379	-E-02		-E-01	0.1410	-0.090
0.1857	-0.0007		+E-03	0.1552	0		-E-01	0.1923	-0.080
0.1870	-0.0006		+E-03	0.3103	+E-02		-E-01	0.2564	-0.070
0.1882	-0.0005		+E-03	0.8966	+E-01		-E-01	0.3333	-0.060
0.1917	-0.0004		+E-03	1.0000	+E 00		-E-01	0.4103	-0.050
0.1942	-0.0003		+E-02	0.0069	-E+01		-E-01	0.5128	-0.040
0.1964	-0.0002		+E-02	0.0278	-E 00		-E-01	0.6026	-0.030
0.2011	-0.0001		+E-02	0.0556	-E-01		-E-01	0.7821	-0.020
0.2012	0.		+E-02	0.0625	-E-02		-E-01	1.0000	-0.010
0.8949	0.		+E-02	0.1528	+E-01		-E-02	0.	-0.010
0.8950	0.0001		+E-02	0.9653	+E 00		-E-02	0.0588	-0.009
0.9002	0.0002		+E-02	1.0000	+E+01		-E-02	0.1765	-0.008
0.9034	0.0003		+E-01	0.0152	-E 00		-E-02	0.2353	-0.007
0.9056	0.0004		+E-01	0.0227	-E-01		-E-02	0.3529	-0.006
0.9062	0.0005		+E-01	0.0303	+E-01		-E-02	0.4118	-0.005
0.9075	0.0006		+E-01	0.2576	+E 00		-E-02	0.5882	-0.003
0.9090	0.0007		+E-01	1.0000	+E+01		-E-02	0.7059	-0.002
0.9109	0.0008						-E-02	1.0000	-0.001
0.9125	0.0009						+E-02	0.	0.001
0.9131	0.0010						+E-02	0.2105	0.002
0.9223	0.0020						+E-02	0.3158	0.003
0.9276	0.0030						+E-02	0.4737	0.006
0.9333	0.0040						+E-02	0.6316	0.007
0.9392	0.0050						+E-02	0.6842	0.008
0.9430	0.0060						+E-02	0.7895	0.009
0.9471	0.0070						+E-02	1.0000	0.010
0.9518	0.0080						+E-01	0.	0.010
0.9562	0.0090						+E-01	0.1525	0.020
0.9585	0.0100						+E-01	0.3559	0.030
0.9792	0.0200						+E-01	0.4407	0.040
0.9868	0.0300						+E-01	0.4915	0.050
0.9931	0.0400						+E-01	0.5593	0.060
0.9972	0.0500						+E-01	0.6441	0.070
0.9987	0.0600						+E-01	0.7797	0.080
0.9994	0.0700						+E-01	0.9153	0.090
0.9997	0.0800						+E-01	1.0000	0.100
1.0000	0.0900						+E 00	0.	0.100
							+E 00	0.2048	0.200
							+E 00	0.3614	0.300
							+E 00	0.4940	0.400
							+E 00	0.6506	0.500
							+E 00	0.7410	0.600
							+E 00	0.8072	0.700
							+E 00	0.8735	0.800
							+E 00	0.9458	0.900
							+E 00	1.0000	1.000
							+E+01	0.	1.000
							+E+01	0.5340	2.000
							+E+01	0.7961	3.000
							+E+01	0.9126	4.000
							+E+01	0.9806	5.000
							+E+01	0.9903	6.000
							+E+01	1.0000	7.000

SET 15 HBC = (0.9000)DE , MBC2 = 0. , T = 1800.

ZH	DELHBC	*	DELHBC RANGE	ZHM	DELMBC2	*	DELMBC2 RANGE	ZM	DELMBC2
******	*******	*	*****	******	*****	*	*****	******	*******
0.	-0.0900		-E-01	0.0112	+E-02		+E-02	0.	0.001
0.0004	-0.0800		-E-01	0.1236	+E-01		+E-02	0.2489	0.002
0.0016	-0.0700		-E-01	0.6292	+E 00		+E-02	0.3846	0.003
0.0037	-0.0500		-E-01	1.0000	+E+01		+E-02	0.5023	0.004
0.0053	-0.0400		-E-02	0.0438	0		+E-02	0.6154	0.005
0.0111	-0.0300		-E-02	0.1825	+E-02		+E-02	0.7104	0.006
0.0184	-0.0200		-E-02	0.4088	+E-01		+E-02	0.7964	0.007
0.0364	-0.0100		-E-02	0.8978	+E 00		+E-02	0.8869	0.008
0.0389	-0.0090		-E-02	1.0000	+E+01		+E-02	0.9457	0.009
0.0409	-0.0080		-E-03	0.2000	0		+E-02	1.0000	0.010
0.0450	-0.0070		-E-03	0.6909	+E-02		+E-01	0.	0.010
0.0483	-0.0060		-E-03	0.8455	+E-01		+E-01	0.3927	0.020
0.0524	-0.0050		-E-03	0.9545	+E 00		+E-01	0.5183	0.030
0.0585	-0.0040		-E-03	1.0000	+E+01		+E-01	0.6492	0.040
0.0639	-0.0030		0	0.9143	0		+E-01	0.7120	0.050
0.0741	-0.0020		0	0.9694	+E-02		+E-01	0.7592	0.060
0.0925	-0.0010		0	0.9975	+E-01		+E-01	0.8010	0.070
0.0954	-0.0009		0	1.0000	+E 00		+E-01	0.8743	0.080
0.0962	-0.0008		+E-03	0.1197	0		+E-01	0.9319	0.090
0.0970	-0.0007		+E-03	0.4951	+E-02		+E-01	1.0000	0.100
0.1003	-0.0006		+E-03	0.8632	+E-01		+E 00	0.	0.100
0.1044	-0.0005		+E-03	0.9829	+E 00		+E 00	0.2248	0.200
0.1105	-0.0004		+E-03	1.0000	+E+01		+E 00	0.3941	0.300
0.1195	-0.0003		+E-02	0.0140	0		+E 00	0.5081	0.400
0.1248	-0.0002		+E-02	0.0791	+E-02		+E 00	0.6417	0.500
0.1375	-0.0001		+E-02	0.2605	+E-01		+E 00	0.7329	0.600
0.1376	0.		+E-02	0.7953	+E 00		+E 00	0.8078	0.700
0.7921	0.		+E-02	1.0000	+E+01		+E 00	0.8892	0.800
0.7922	0.0001		+E-01	0.0057	+E-02		+E 00	0.9316	0.900
0.8101	0.0002		+E-01	0.0398	+E-01		+E 00	1.0000	1.000
0.8207	0.0003		+E-01	0.3239	+E 00		+E+01	0.	1.000
0.8256	0.0004		+E-01	1.0000	+E+01		+E+01	0.4747	2.000
0.8297	0.0005						+E+01	0.6774	3.000
0.8330	0.0006						+E+01	0.7926	4.000
0.8334	0.0007						+E+01	0.8986	5.000
0.8342	0.0008						+E+01	0.9585	6.000
0.8359	0.0009						+E+01	0.9677	7.000
0.8400	0.0010						+E+01	0.9908	8.000
0.8580	0.0020						+E+01	0.9954	9.000
0.8702	0.0030						+E+01	1.0000	10.000
0.8805	0.0040								
0.8862	0.0050								
0.8968	0.0060								
0.9038	0.0070								
0.9099	0.0080								
0.9190	0.0090								
0.9280	0.0100								
0.9652	0.0200								
0.9828	0.0300								
0.9926	0.0400								
0.9963	0.0500								
0.9984	0.0600								
0.9992	0.0700								
0.9996	0.0800								
1.0000	0.1000								

SET 16 HBC = (0.9000)DE , MBC2 = 0.01 , T = 1800.

ZH	DELHBC	*	DELHBC RANGE	ZHM	DELMBC2 RANGE	*	DELMBC2 RANGE	ZM	DELMBC2
******	*******	*	*****	******	*****	*	*****	******	*******
0.	-0.1000		-E-01	0.0208	-E-02		-E-02	0.	-0.010
0.0008	-0.0900		-E-01	0.0312	+E-02		-E-02	0.0863	-0.009
0.0012	-0.0800		-E-01	0.1354	+E-01		-E-02	0.1871	-0.008
0.0016	-0.0700		-E-01	0.5729	+E 00		-E-02	0.2662	-0.007
0.0028	-0.0600		-E-01	1.0000	+E+01		-E-02	0.3741	-0.006
0.0036	-0.0500		-E-02	0.0699	-E-02		-E-02	0.5252	-0.005
0.0056	-0.0400		-E-02	0.0909	0		-E-02	0.6475	-0.004
0.0120	-0.0300		-E-02	0.1748	+E-02		-E-02	0.7770	-0.003
0.0195	-0.0200		-E-02	0.4476	+E-01		-E-02	0.8705	-0.002
0.0383	-0.0100		-E-02	0.8951	+E 00		-E-02	1.0000	-0.001
0.0403	-0.0090		-E-02	1.0000	+E+01		+E-02	0.	0.001
0.0435	-0.0080		-E-03	0.3551	-E-02		+E-02	0.1565	0.002
0.0487	-0.0070		-E-03	0.4203	0		+E-02	0.3043	0.003
0.0527	-0.0060		-E-03	0.6232	+E-02		+E-02	0.4261	0.004
0.0546	-0.0050		-E-03	0.8261	+E-01		+E-02	0.4957	0.005
0.0586	-0.0040		-E-03	0.9638	+E 00		+E-02	0.6348	0.006
0.0666	-0.0030		-E-03	1.0000	+E+01		+E-02	0.7739	0.007
0.0782	-0.0020		0	0.0305	-E-02		+E-02	0.8261	0.008
0.0953	-0.0010		0	0.9561	0		+E-02	0.9130	0.009
0.0989	-0.0009		0	0.9799	+E-02		+E-02	1.0000	0.010
0.1017	-0.0008		0	0.9963	+E-01		+E-01	0.	0.010
0.1025	-0.0007		0	0.9994	+E 00		+E-01	0.3682	0.020
0.1049	-0.0006		0	1.0000	+E+01		+E-01	0.5423	0.030
0.1097	-0.0005		+E-03	0.1719	-E-02		+E-01	0.6468	0.040
0.1141	-0.0004		+E-03	0.2109	0		+E-01	0.7164	0.050
0.1205	-0.0003		+E-03	0.3984	+E-02		+E-01	0.8507	0.060
0.1300	-0.0002		+E-03	0.8906	+E-01		+E-01	0.9104	0.070
0.1504	-0.0001		+E-03	0.9688	+E 00		+E-01	0.9303	0.080
0.1505	0.		+E-03	1.0000	+E+01		+E-01	0.9751	0.090
0.8041	0.		+E-02	0.0191	-E-02		+E-01	1.0000	0.100
0.8042	0.0001		+E-02	0.0239	0		+E 00	0.	0.100
0.8221	0.0002		+E-02	0.0718	+E-02		+E 00	0.2458	0.200
0.8289	0.0003		+E-02	0.2153	+E-01		+E 00	0.4209	0.300
0.8392	0.0004		+E-02	0.7464	+E 00		+E 00	0.5690	0.400
0.8424	0.0005		+E-02	1.0000	+E+01		+E 00	0.6734	0.500
0.8452	0.0006		+E-01	0.0130	-E-02		+E 00	0.7441	0.600
0.8476	0.0007		+E-01	0.0195	+E-02		+E 00	0.8215	0.700
0.8516	0.0008		+E-01	0.0455	+E-01		+E 00	0.8923	0.800
0.8540	0.0009		+E-01	0.3442	+E 00		+E 00	0.9495	0.900
0.8552	0.0010		+E-01	1.0000	+E+01		+E 00	1.0000	1.000
0.8736	0.0020						+E+01	0.	1.000
0.8871	0.0030						+E+01	0.4955	2.000
0.8963	0.0040						+E+01	0.7364	3.000
0.9031	0.0050						+E+01	0.8318	4.000
0.9095	0.0060						+E+01	0.9227	5.000
0.9174	0.0070						+E+01	0.9727	6.000
0.9290	0.0080						+E+01	0.9909	7.000
0.9350	0.0090						+E+01	1.0000	8.000
0.9386	0.0100								
0.9753	0.0200								
0.9944	0.0300								
0.9984	0.0400								
1.0000	0.0500								

SET 17 . HBC = (0.9000)DE , MBC2 = 0.10 , T = 1800.

ZH	DELHBC	*	DELHBC RANGE	ZHM	DELMBC2 RANGE	*	DELMBC2 RANGE	ZM	DELMBC2
******	*******	*	*****	******	*****	*	*****	******	*******
0.	-0.2000		-E 00	1.0000	+E 00		-E-01	0.	-0.100
0.0004	-0.1000		-E-01	0.0625	-E-01		-E-01	0.0398	-0.090
0.0008	-0.0900		-E-01	0.0729	-E-02		-E-01	0.0995	-0.080
0.0012	-0.0800		-E-01	0.0833	0		-E-01	0.1642	-0.070
0.0028	-0.0600		-E-01	0.1042	+E-02		-E-01	0.2139	-0.060
0.0040	-0.0500		-E-01	0.1562	+E-01		-E-01	0.3035	-0.050
0.0044	-0.0400		-E-01	0.5729	+E 00		-E-01	0.4129	-0.040
0.0111	-0.0300		-E-01	1.0000	+E+01		-E-01	0.6219	-0.030
0.0191	-0.0200		-E-02	0.2252	-E-01		-E-01	0.7463	-0.020
0.0385	-0.0100		-E-02	0.2649	-E-02		-E-01	1.0000	-0.010
0.0437	-0.0090		-E-02	0.2914	0		-E-02	0.	-0.010
0.0473	-0.0080		-E-02	0.3444	+E-02		-E-02	0.1522	-0.009
0.0509	-0.0070		-E-02	0.4901	+E-01		-E-02	0.2391	-0.008
0.0548	-0.0060		-E-02	0.8543	+E 00		-E-02	0.3913	-0.007
0.0572	-0.0050		-E-02	1.0000	+E+01		-E-02	0.4783	-0.006
0.0663	-0.0040		-E-03	0.6292	-E-01		-E-02	0.6522	-0.005
0.0731	-0.0030		-E-03	0.7191	-E-02		-E-02	0.7609	-0.004
0.0803	-0.0020		-E-03	0.7472	0		-E-02	0.8696	-0.003
0.0985	-0.0010		-E-03	0.8034	+E-02		-E-02	0.9348	-0.002
0.1017	-0.0009		-E-03	0.9213	+E-01		-E-02	1.0000	-0.001
0.1045	-0.0008		-E-03	0.9944	+E 00		+E-02	0.	0.001
0.1081	-0.0007		-E-03	1.0000	+E+01		+E-02	0.2000	0.002
0.1124	-0.0006		0	0.0089	-E-01		+E-02	0.3000	0.003
0.1192	-0.0005		0	0.0159	-E-02		+E-02	0.3750	0.004
0.1271	-0.0004		0	0.9835	0		+E-02	0.5000	0.005
0.1398	-0.0003		0	0.9892	+E-02		+E-02	0.6750	0.006
0.1549	-0.0002		0	0.9987	+E-01		+E-02	0.7500	0.007
0.1692	-0.0001		0	1.0000	+E 00		+E-02	0.7750	0.008
0.1693	0.		+E-03	0.1039	-E-01		+E-02	0.8750	0.009
0.7946	0.		+E-03	0.1429	-E-02		+E-02	1.0000	0.010
0.7947	0.0001		+E-03	0.1494	0		+E-01	0.	0.010
0.8077	0.0002		+E-03	0.2013	+E-02		+E-01	0.2324	0.020
0.8160	0.0003		+E-03	0.8377	+E-01		+E-01	0.3838	0.030
0.8256	0.0004		+E-03	0.9870	+E 00		+E-01	0.5081	0.040
0.8319	0.0005		+E-03	1.0000	+E+01		+E-01	0.6378	0.050
0.8375	0.0006		+E-02	0.0680	-E-01		+E-01	0.7730	0.060
0.8435	0.0007		+E-02	0.0971	-E-02		+E-01	0.8270	0.070
0.8502	0.0008		+E-02	0.1117	+E-02		+E-01	0.8973	0.080
0.8530	0.0009		+E-02	0.2039	+E-01		+E-01	0.9676	0.090
0.8558	0.0010		+E-02	0.7670	+E 00		+E-01	1.0000	0.100
0.8729	0.0020		+E-02	1.0000	+E+01		+E 00	0.	0.100
0.8864	0.0030		+E-01	0.0318	-E-01		+E 00	0.2189	0.200
0.8963	0.0040		+E-01	0.0637	+E-01		+E 00	0.4007	0.300
0.9050	0.0050		+E-01	0.3631	+E 00		+E 00	0.5051	0.400
0.9158	0.0060		+E-01	1.0000	+E+01		+E 00	0.6027	0.500
0.9225	0.0070						+E 00	0.7037	0.600
0.9261	0.0080						+E 00	0.7946	0.700
0.9317	0.0090						+E 00	0.8687	0.800
0.9376	0.0100						+E 00	0.9327	0.900
0.9770	0.0200						+E 00	1.0000	1.000
0.9928	0.0300						+E+01	0.	1.000
0.9980	0.0400						+E+01	0.4953	2.000
0.9996	0.0500						+E+01	0.6963	3.000
1.0000	0.0600						+E+01	0.8364	4.000
							+E+01	0.9112	5.000
							+E+01	0.9676	6.000
							+E+01	0.9907	7.000
							+E+01	1.0000	8.000

SET 18 HBC = (0.9000)DE , MBC2 = 1.00 , T = 1800.

ZH	DELHBC	*	DELHBC RANGE	ZHM	DELMBC2	*	DELMBC2 RANGE	ZM	DELMBC2
******	*******	*	*****	******	*****	*	*****	******	*******
0.	-0.2000		-E 00	0.5000	+E 00		-E 00	0.	-1.000
0.0008	-0.1000		-E 00	1.0000	+E+01		-E 00	0.0883	-0.900
0.0020	-0.0800		-E-01	0.5091	-E 00		-E 00	0.1661	-0.800
0.0031	-0.0700		-E-01	0.5455	-E-01		-E 00	0.2438	-0.700
0.0035	-0.0600		-E-01	0.5546	+E-02		-E 00	0.3357	-0.600
0.0043	-0.0500		-E-01	0.6091	+E-01		-E 00	0.4134	-0.500
0.0071	-0.0400		-E-01	0.7636	+E 00		-E 00	0.4912	-0.400
0.0133	-0.0300		-E-01	1.0000	+E+01		-E 00	0.6042	-0.300
0.0243	-0.0200		-E-02	0.6822	-E 00		-E 00	0.7527	-0.200
0.0439	-0.0100		-E-02	0.7664	-E-01		-E 00	1.0000	-0.100
0.0462	-0.0090		-E-02	0.7710	-E-02		-E-01	0.	-0.100
0.0529	-0.0080		-E-02	0.7757	0		-E-01	0.0840	-0.090
0.0553	-0.0070		-E-02	0.8318	+E-01		-E-01	0.1513	-0.080
0.0647	-0.0060		-E-02	0.9393	+E 00		-E-01	0.2857	-0.070
0.0701	-0.0050		-E-02	1.0000	+E+01		-E-01	0.4034	-0.060
0.0780	-0.0040		-E-03	0.1883	-E 00		-E-01	0.4958	-0.050
0.0858	-0.0030		-E-03	0.6818	-E-01		-E-01	0.5966	-0.040
0.0991	-0.0020		-E-03	0.7597	-E-02		-E-01	0.7227	-0.030
0.1277	-0.0010		-E-03	0.7727	0		-E-01	0.8319	-0.020
0.1324	-0.0009		-E-03	0.8052	+E-02		-E-01	1.0000	-0.010
0.1348	-0.0008		-E-03	0.9156	+E-01		-E-02	0.	-0.009
0.1399	-0.0007		-E-03	0.9870	+E 00		-E-02	0.1500	-0.008
0.1489	-0.0006		-E-03	1.0000	+E+01		-E-02	0.2500	-0.007
0.1540	-0.0005		0	0.0006	-E 00		-E-02	0.3000	-0.006
0.1626	-0.0004		0	0.0044	-E-01		-E-02	0.5500	-0.005
0.1728	-0.0003		0	0.0051	-E-02		-E-02	0.6500	-0.004
0.1799	-0.0002		0	0.9911	0		-E-02	0.7000	-0.003
0.1881	-0.0001		0	0.9924	+E-02		-E-02	0.7500	-0.002
0.1882	0.		0	0.9975	+E-01		-E-02	1.0000	-0.001
0.8053	0.		0	0.9987	+E 00		+E-02	0.	0.001
0.8054	0.0001		0	1.0000	+E+01		+E-02	0.3000	0.002
0.8135	0.0002		+E-03	0.0885	-E 00		+E-02	0.4000	0.003
0.8178	0.0003		+E-03	0.1770	-E-01		+E-02	0.5000	0.004
0.8241	0.0004		+E-03	0.2124	-E-02		+E-02	0.7000	0.005
0.8280	0.0005		+E-03	0.2301	+E-02		+E-02	0.8000	0.007
0.8311	0.0006		+E-03	0.7611	+E-01		+E-02	0.9000	0.009
0.8346	0.0007		+E-03	0.9912	+E 00		+E-02	1.0000	0.010
0.8386	0.0008		+E-03	1.0000	+E+01		+E-01	0.	0.010
0.8444	0.0009		+E-02	0.1471	-E 00		+E-01	0.1803	0.020
0.8495	0.0010		+E-02	0.1618	-E-01		+E-01	0.2623	0.030
0.8703	0.0020		+E-02	0.1667	-E-02		+E-01	0.4016	0.040
0.8797	0.0030		+E-02	0.1716	0		+E-01	0.5082	0.050
0.8879	0.0040		+E-02	0.2304	+E-01		+E-01	0.6393	0.060
0.8958	0.0050		+E-02	0.7304	+E 00		+E-01	0.7705	0.070
0.9052	0.0060		+E-02	1.0000	+E+01		+E-01	0.8361	0.080
0.9111	0.0070		+E-01	0.0611	-E 00		+E-01	0.9344	0.090
0.9177	0.0080		+E-01	0.0722	-E-01		+E-01	1.0000	0.100
0.9220	0.0090		+E-01	0.0778	-E-02		+E 00	0.	0.100
0.9295	0.0100		+E-01	0.1167	+E-01		+E 00	0.3073	0.200
0.9687	0.0200		+E-01	0.3167	+E 00		+E 00	0.4450	0.300
0.9914	0.0300		+E-01	1.0000	+E+01		+E 00	0.5780	0.400
0.9976	0.0400						+E 00	0.6376	0.500
1.0000	0.0500						+E 00	0.7248	0.600
							+E 00	0.8119	0.700
							+E 00	0.8853	0.800
							+E 00	0.9450	0.900
							+E 00	1.0000	1.000
							+E+01	0.	1.000
							+E+01	0.4215	2.000
							+E+01	0.5964	3.000
							+E+01	0.7534	4.000
							+E+01	0.8565	5.000
							+E+01	0.9148	6.000
							+E+01	0.9686	7.000
							+E+01	0.9821	8.000
							+E+01	1.0000	9.000

SET 19 HBC = (0.9000)DE , MBC2 = 2.00 , T = 1800.

ZH	DELHBC	*	DELHBC RANGE	ZHM	DELMBC2 RANGE	*	DELMBC2 RANGE	ZM	DELMBC2
******	*******	*	*****	******	*****	*	*****	******	*******
0.	-0.2000		-E 00	0.5000	+E-01		-E+01	0.	-2.000
0.0008	-0.1000		-E 00	1.0000	+E+01		-E+01	1.0000	-1.000
0.0015	-0.0700		-E-01	0.4588	-E+01		-E 00	0.	-1.000
0.0031	-0.0600		-E-01	0.7353	-E 00		-E 00	0.0728	-0.900
0.0046	-0.0500		-E-01	0.7588	-E-01		-E 00	0.1068	-0.800
0.0096	-0.0400		-E-01	0.7647	+E-02		-E 00	0.1893	-0.700
0.0192	-0.0300		-E-01	0.7824	+E-01		-E 00	0.2330	-0.600
0.0338	-0.0200		-E-01	0.9000	+E 00		-E 00	0.3495	-0.500
0.0661	-0.0100		-E-01	1.0000	+E+01		-E 00	0.4903	-0.400
0.0711	-0.0090		-E-02	0.1990	-E+01		-E 00	0.6311	-0.300
0.0761	-0.0080		-E-02	0.6893	-E 00		-E 00	0.7816	-0.200
0.0807	-0.0070		-E-02	0.7573	-E-01		-E 00	1.0000	-0.100
0.0864	-0.0060		-E-02	0.7621	-E-02		-E-01	0.	-0.100
0.0937	-0.0050		-E-02	0.8204	+E-01		-E-01	0.1111	-0.090
0.1030	-0.0040		-E-02	0.9515	+E 00		-E-01	0.2407	-0.080
0.1114	-0.0030		-E-02	1.0000	+E+01		-E-01	0.3333	-0.070
0.1233	-0.0020		-E-03	0.0926	-E 00		-E-01	0.3704	-0.060
0.1452	-0.0010		-E-03	0.6852	-E-01		-E-01	0.5370	-0.050
0.1468	-0.0009		-E-03	0.7500	-E-02		-E-01	0.6204	-0.040
0.1502	-0.0008		-E-03	0.7593	0		-E-01	0.7037	-0.030
0.1529	-0.0007		-E-03	0.8333	+E-02		-E-01	0.8333	-0.020
0.1567	-0.0006		-E-03	0.9352	+E-01		-E-01	1.0000	-0.010
0.1617	-0.0005		-E-03	0.9907	+E 00		-E-02	0.	-0.009
0.1702	-0.0004		-E-03	1.0000	+E+01		-E-02	0.0714	-0.008
0.1744	-0.0003		0	0.0018	-E 00		-E-02	0.3571	-0.007
0.1798	-0.0002		0	0.0080	-E-01		-E-02	0.5714	-0.006
0.1867	-0.0001		0	0.0098	-E-02		-E-02	0.7143	-0.005
0.1868	0.		0	0.9926	0		-E-02	0.9286	-0.003
0.8133	0.		0	0.9939	+E-02		-E-02	1.0000	-0.001
0.8134	0.0001		0	0.9988	+E-01		+E-02	0.	0.001
0.8179	0.0002		0	0.9994	+E 00		+E-02	0.1818	0.002
0.8206	0.0003		0	1.0000	+E+01		+E-02	0.2727	0.004
0.8267	0.0004		+E-03	0.1000	-E 00		+E-02	0.3636	0.005
0.8313	0.0005		+E-03	0.1333	-E-01		+E-02	0.5455	0.006
0.8356	0.0006		+E-03	0.1444	-E-02		+E-02	0.7273	0.007
0.8383	0.0007		+E-03	0.7778	+E-01		+E-02	0.9091	0.008
0.8425	0.0008		+E-03	0.9889	+E 00		+E-02	1.0000	0.009
0.8456	0.0009		+E-03	1.0000	+E+01		+E-01	0.	0.010
0.8479	0.0010		+E-02	0.0461	-E+01		+E-01	0.1650	0.020
0.8725	0.0020		+E-02	0.1659	-E 00		+E-01	0.3010	0.030
0.8844	0.0030		+E-02	0.2120	-E-01		+E-01	0.4078	0.040
0.8936	0.0040		+E-02	0.2166	-E-02		+E-01	0.4951	0.050
0.9032	0.0050		+E-02	0.2581	+E-01		+E-01	0.6408	0.060
0.9090	0.0060		+E-02	0.7788	+E 00		+E-01	0.7184	0.070
0.9147	0.0070		+E-02	1.0000	+E+01		+E-01	0.8350	0.080
0.9209	0.0080		+E-01	0.0279	-E+01		+E-01	0.9125	0.090
0.9274	0.0090		+E-01	0.0838	-E 00		+E-01	1.0000	0.100
0.9312	0.0100		+E-01	0.1006	-E-01		+E 00	0.	0.100
0.9681	0.0200		+E-01	0.1061	-E-02		+E 00	0.2453	0.200
0.9885	0.0300		+E-01	0.1173	+E-01		+E 00	0.4292	0.300
0.9954	0.0400		+E-01	0.2626	+E 00		+E 00	0.5802	0.400
0.9992	0.0500		+E-01	0.9777	+E+01		+E 00	0.6981	0.500
0.9996	0.0600		+E-01	1.0000	+E+02		+E 00	0.7736	0.600
1.0000	0.0700						+E 00	0.8632	0.700
							+E 00	0.9292	0.800
							+E 00	0.9623	0.900
							+E 00	1.0000	1.000
							+E+01	0.	1.000
							+E+01	0.4444	2.000
							+E+01	0.6570	3.000
							+E+01	0.7826	4.000
							+E+01	0.8261	5.000
							+E+01	0.8986	6.000
							+E+01	0.9614	7.000
							+E+01	0.9903	8.000
							+E+01	1.0000	10.000
							+E+02	0.	10.000
							+E+02	1.0000	20.000

SET 20 HBC = (0.9000)DE , MBC2 = 5.00 , T = 1800.

ZH	DELHBC	*	DELHBC RANGE	ZHM	DELMBC2	*	DELMBC2 RANGE	ZM	DELMBC2
******	*******	*	*****	******	*****	*	*****	******	*******
0.	-0.2000		-E 00	1.0000	-E+01		-E+01	0.	-5.000
0.0018	-0.1000		-E-01	0.7188	-E+01		-E+01	0.1100	-4.000
0.0029	-0.0900		-E-01	0.8658	-E 00		-E+01	0.3300	-3.000
0.0040	-0.0800		-E-01	0.8786	-E-01		-E+01	0.5500	-2.000
0.0063	-0.0700		-E-01	0.8818	+E-02		-E+01	1.0000	-1.000
0.0096	-0.0600		-E-01	0.8914	+E-01		-E 00	0.	-1.000
0.0177	-0.0500		-E-01	0.9329	+E 00		-E 00	0.0635	-0.900
0.0280	-0.0400		-E-01	1.0000	+E+01		-E 00	0.1587	-0.800
0.0471	-0.0300		-E-02	0.2328	-E+01		-E 00	0.2011	-0.700
0.0743	-0.0200		-E-02	0.6878	-E 00		-E 00	0.2804	-0.600
0.1170	-0.0100		-E-02	0.7302	-E-01		-E 00	0.3598	-0.500
0.1236	-0.0090		-E-02	0.7354	-E-02		-E 00	0.4603	-0.400
0.1280	-0.0080		-E-02	0.7407	+E-02		-E 00	0.6243	-0.300
0.1321	-0.0070		-E-02	0.7779	+E-01		-E 00	0.7937	-0.200
0.1376	-0.0060		-E-02	0.9418	+E 00		-E 00	1.0000	-0.100
0.1453	-0.0050		-E-02	1.0000	+E+01		-E-01	0.	-0.100
0.1508	-0.0040		-E-03	0.0128	-E+01		-E-01	0.1081	-0.090
0.1586	-0.0030		-E-03	0.1923	-E 00		-E-01	0.1622	-0.080
0.1681	-0.0020		-E-03	0.6538	-E-01		-E-01	0.2432	-0.070
0.1865	-0.0010		-E-03	0.7564	-E-02		-E-01	0.3108	-0.060
0.1884	-0.0009		-E-03	0.8077	+E-02		-E-01	0.4865	-0.050
0.1917	-0.0008		-E-03	0.9103	+E-01		-E-01	0.6216	-0.040
0.1946	-0.0007		-E-03	0.9872	+E 00		-E-01	0.7973	-0.030
0.1965	-0.0006		-E-03	1.0000	+E+01		-E-01	0.9324	-0.020
0.2009	-0.0005		0	0.0006	-E 00		-E-01	1.0000	-0.010
0.2035	-0.0004		0	0.0052	-E-01		-E-02	0.	-0.010
0.2064	-0.0003		0	0.0080	-E-02		-E-02	0.0588	-0.009
0.2090	-0.0002		0	0.9914	0		-E-02	0.4118	-0.008
0.2152	-0.0001		0	0.9926	+E-02		-E-02	0.5294	-0.007
0.2153	0.		0	0.9989	+E-01		-E-02	0.7059	-0.006
0.8580	0.		0	1.0000	+E 00		-E-02	0.8235	-0.004
0.8581	0.0001		+E-03	0.0323	-E+01		-E-02	0.9412	-0.003
0.8609	0.0002		+E-03	0.1935	-E 00		-E-02	1.0000	-0.001
0.8657	0.0003		+E-03	0.3065	-E-01		+E-02	0.	0.002
0.8675	0.0004		+E-03	0.3548	-E-02		+E-02	0.2857	0.003
0.8720	0.0005		+E-03	0.3710	0		+E-02	0.3571	0.004
0.8753	0.0006		+E-03	0.4194	+E-02		+E-02	0.5714	0.005
0.8775	0.0007		+E-03	0.8226	+E-01		+E-02	0.7143	0.006
0.8782	0.0008		+E-03	0.9677	+E 00		+E-02	0.7857	0.007
0.8793	0.0009		+E-03	1.0000	+E+01		+E-02	0.9286	0.009
0.8808	0.0010		+E-02	0.0747	-E+01		+E-02	1.0000	0.010
0.9010	0.0020		+E-02	0.2011	-E 00		+E-01	0.	0.010
0.9110	0.0030		+E-02	0.2586	-E-01		+E-01	0.1719	0.020
0.9176	0.0040		+E-02	0.2759	+E-02		+E-01	0.3125	0.030
0.9249	0.0050		+E-02	0.3333	+E-01		+E-01	0.4844	0.040
0.9308	0.0060		+E-02	0.8391	+E 00		+E-01	0.6250	0.050
0.9338	0.0070		+E-02	1.0000	+E+01		+E-01	0.7344	0.060
0.9378	0.0080		+E-01	0.0671	-E+01		+E-01	0.8281	0.070
0.9411	0.0090		+E-01	0.1342	-E 00		+E-01	0.8750	0.080
0.9448	0.0100		+E-01	0.1409	-E-01		+E-01	0.9375	0.090
0.9713	0.0200		+E-01	0.2886	+E 00		+E-01	1.0000	0.100
0.9823	0.0300		+E-01	0.9530	+E+01		+E 00	0.	0.100
0.9912	0.0400		+E-01	1.0000	+E+02		+E 00	0.3041	0.200
0.9948	0.0500		+E 00	1.0000	+E+02		+E 00	0.4620	0.300
0.9978	0.0600						+E 00	0.5848	0.400
0.9990	0.0800						+E 00	0.6550	0.500
0.9993	0.0900						+E 00	0.7602	0.600
0.9996	0.1000						+E 00	0.8421	0.700
1.0000	0.2000						+E 00	0.8889	0.800
							+E 00	0.9298	0.900
							+E 00	1.0000	1.000
							+E+01	0.	1.000
							+E+01	0.4691	2.000
							+E+01	0.7222	3.000
							+E+01	0.8395	4.000
							+E+01	0.9074	5.000
							+E+01	0.9259	6.000
							+E+01	0.9321	7.000
							+E+01	0.9630	8.000
							+E+01	0.9877	9.000
							+E+01	1.0000	10.000
							+E+02	0.	10.000
							+E+02	1.0000	20.000

SET 21 MBC = (0.9000)DE , MBC2 = 10.00 , T = 1800.

ZH	DELMBC	*	DELMBC RANGE	ZHM	DELMBC2 RANGE	*	DELMBC2 RANGE	ZM	DELMBC2
******	*******	*	*****	******	*****	*	*****	******	*******
0.	-0.2000		-E 00	1.0000	-E+01		-E+01	0.	-10.000
0.0150	-0.1000		-E-01	0.8473	-E+01		-E+01	0.0138	-9.000
0.0204	-0.0900		-E-01	0.9507	-E 00		-E+01	0.0528	-8.000
0.0255	-0.0800		-E-01	0.9532	-E-01		-E+01	0.1009	-7.000
0.0326	-0.0700		-E-01	0.9557	+E-01		-E+01	0.1789	-6.000
0.0425	-0.0600		-E-01	0.9926	+E 00		-E+01	0.3005	-5.000
0.0567	-0.0500		-E-01	1.0000	+E+01		-E+01	0.4541	-4.000
0.0748	-0.0400		-E-02	0.2067	-E+01		-E+01	0.5849	-3.000
0.0951	-0.0300		-E-02	0.6400	-E 00		-E+01	0.7638	-2.000
0.1240	-0.0200		-E-02	0.7267	-E-01		-E+01	1.0000	-1.000
0.1529	-0.0100		-E-02	0.7333	-E-02		-E 00	0.	-1.000
0.1583	-0.0090		-E-02	0.7400	+E-01		-E 00	0.1560	-0.900
0.1624	-0.0080		-E-02	0.8733	+E 00		-E 00	0.2057	-0.800
0.1665	-0.0070		-E-02	1.0000	+E+01		-E 00	0.3191	-0.700
0.1702	-0.0060		-E-03	0.0147	-E+01		-E 00	0.4255	-0.600
0.1760	-0.0050		-E-03	0.1618	-E 00		-E 00	0.5390	-0.500
0.1821	-0.0040		-E-03	0.6029	-E-01		-E 00	0.6454	-0.400
0.1876	-0.0030		-E-03	0.6912	-E-02		-E 00	0.7234	-0.300
0.1954	-0.0020		-E-03	0.7206	0		-E 00	0.8085	-0.200
0.2039	-0.0010		-E-03	0.8088	+E-02		-E 00	1.0000	-0.100
0.2052	-0.0009		-E-03	0.8824	+E-01		-E-01	0.	-0.100
0.2059	-0.0008		-E-03	0.9706	+E 00		-E-01	0.1186	-0.090
0.2073	-0.0007		-E-03	1.0000	+E+01		-E-01	0.2203	-0.080
0.2086	-0.0006		0	0.0010	-E 00		-E-01	0.3559	-0.070
0.2120	-0.0005		0	0.0025	-E-01		-E-01	0.4746	-0.060
0.2154	-0.0004		0	0.0056	-E-02		-E-01	0.5424	-0.050
0.2192	-0.0003		0	0.9919	0		-E-01	0.6102	-0.040
0.2236	-0.0002		0	0.9939	+E-02		-E-01	0.7288	-0.030
0.2270	-0.0001		0	0.9995	+E-01		-E-01	0.9153	-0.020
0.2271	0.		0	1.0000	+E 00		-E-01	1.0000	-0.010
0.8967	0.		+E-03	0.0615	-E-01		-E-02	0.	-0.010
0.8968	0.0001		+E-03	0.0769	-E-02		-E-02	0.0667	-0.009
0.8998	0.0002		+E-03	0.0923	+E-02		-E-02	0.1333	-0.008
0.9032	0.0003		+E-03	0.7692	+E-01		-E-02	0.4667	-0.007
0.9059	0.0004		+E-03	1.0000	+E 00		-E-02	0.5333	-0.006
0.9096	0.0005		+E-02	0.0672	-E+01		-E-02	0.7500	-0.005
0.9120	0.0006		+E-02	0.2090	-E 00		-E-02	0.8000	-0.004
0.9123	0.0007		+E-02	0.2612	-E-01		-E-02	0.8667	-0.003
0.9154	0.0008		+E-02	0.2687	-E-02		-E-02	1.0000	-0.001
0.9166	0.0009		+E-02	0.2761	+E-02		+E-02	0.	0.003
0.9188	0.0010		+E-02	0.3507	+E-01		+E-02	0.1667	0.004
0.9290	0.0020		+E-02	0.8657	+E 00		+E-02	0.2500	0.005
0.9354	0.0030		+E-02	1.0000	+E+01		+E-02	0.4167	0.006
0.9426	0.0040		+E-01	0.0667	-E+01		+E-02	0.5000	0.007
0.9497	0.0050		+E-01	0.0952	-E 00		+E-02	0.6667	0.008
0.9541	0.0060		+E-01	0.1048	-E-01		+E-02	0.8333	0.009
0.9572	0.0070		+E-01	0.1238	+E-01		+E-02	1.0000	0.010
0.9602	0.0080		+E-01	0.3048	+E 00		+E-01	0.	0.010
0.9630	0.0090		+E-01	0.9810	+E+01		+E-01	0.1216	0.020
0.9643	0.0100		+E-01	1.0000	+E+02		+E-01	0.3514	0.030
0.9783	0.0200						+E-01	0.5405	0.040
0.9898	0.0300						+E-01	0.6351	0.050
0.9946	0.0400						+E-01	0.7162	0.060
0.9966	0.0500						+E-01	0.8243	0.070
0.9980	0.0600						+E-01	0.8514	0.080
0.9986	0.0700						+E-01	0.8919	0.090
0.9993	0.0800						+E-01	1.0000	0.100
1.0000	0.1000						+E 00	0.	0.100
							+E 00	0.2207	0.200
							+E 00	0.3862	0.300
							+E 00	0.5103	0.400
							+E 00	0.6000	0.500
							+E 00	0.6897	0.600
							+E 00	0.7655	0.700
							+E 00	0.8552	0.800
							+E 00	0.9172	0.900
							+E 00	1.0000	1.000
							+E+01	0.	1.000
							+E+01	0.5310	2.000
							+E+01	0.7611	3.000
							+E+01	0.8673	4.000
							+E+01	0.9381	5.000
							+E+01	0.9823	6.000
							+E+01	1.0000	7.000
							+E+02	0.	10.000
							+E+02	1.0000	20.000

SET 22 HBC = (0.9000)DE , MBC2 = 19.00 , T = 1800.

ZH	DELHBC	*	DELHBC RANGE	ZHM	DELMBC2 RANGE	*	DELMBC2 RANGE	ZM	DELMBC2
******	*******	*	*****	******	*****	*	*****	******	*******
0.	-0.3000		-E 00	0.5051	-E+02		-E+02	0.	-19.000
0.0009	-0.2000		-E 00	1.0000	-E+01		-E+02	1.0000	-10.000
0.0311	-0.1000		-E-01	0.0108	-E+02		-E+01	0.	-10.000
0.0370	-0.0900		-E-01	0.8726	-E+01		-E+01	0.0384	-9.000
0.0408	-0.0800		-E-01	0.9919	-E 00		-E+01	0.1125	-8.000
0.0492	-0.0700		-E-01	0.9973	-E-01		-E+01	0.1918	-7.000
0.0590	-0.0600		-E-01	1.0000	+E 00		-E+01	0.2762	-6.000
0.0703	-0.0500		-E-02	0.1172	-E+01		-E+01	0.3555	-5.000
0.0831	-0.0400		-E-02	0.7724	-E 00		-E+01	0.4476	-4.000
0.0991	-0.0300		-E-02	0.8828	-E-01		-E+01	0.5857	-3.000
0.1195	-0.0200		-E-02	0.9379	+E-01		-E+01	0.7519	-2.000
0.1468	-0.0100		-E-02	0.9862	+E 00		-E+01	1.0000	-1.000
0.1524	-0.0090		-E-02	1.0000	+E+01		-E 00	0.	-1.000
0.1550	-0.0080		-E-03	0.0323	-E+01		-E 00	0.1111	-0.900
0.1575	-0.0070		-E-03	0.1613	-E 00		-E 00	0.1944	-0.800
0.1628	-0.0060		-E-03	0.7258	-E-01		-E 00	0.3278	-0.700
0.1675	-0.0050		-E-03	0.7742	-E-02		-E 00	0.4000	-0.600
0.1722	-0.0040		-E-03	0.9032	+E-01		-E 00	0.4889	-0.500
0.1775	-0.0030		-E-03	1.0000	+E 00		-E 00	0.5722	-0.400
0.1848	-0.0020		0	0.0018	-E-01		-E 00	0.6611	-0.300
0.1923	-0.0010		0	0.0063	-E-02		-E 00	0.7389	-0.200
0.1932	-0.0009		0	0.9937	0		-E 00	1.0000	-0.100
0.1948	-0.0008		0	0.9978	+E-02		-E-01	0.	-0.100
0.1957	-0.0007		0	0.9996	+E-01		-E-01	0.0429	-0.090
0.1976	-0.0006		0	1.0000	+E 00		-E-01	0.1286	-0.080
0.1995	-0.0005		+E-03	0.2000	-E 00		-E-01	0.1857	-0.070
0.2014	-0.0004		+E-03	0.2222	-E-01		-E-01	0.2571	-0.060
0.2048	-0.0003		+E-03	0.2444	-E-02		-E-01	0.3714	-0.050
0.2080	-0.0002		+E-03	0.2667	0		-E-01	0.4571	-0.040
0.2117	-0.0001		+E-03	0.3556	+E-02		-E-01	0.6286	-0.030
0.2118	0.		+E-03	0.8222	+E-01		-E-01	0.8143	-0.020
0.9090	0.		+E-03	1.0000	+E 00		-E-01	1.0000	-0.010
0.9091	0.0001		+E-02	0.0211	-E+01		-E-02	0.	-0.010
0.9109	0.0002		+E-02	0.1831	-E 00		-E-02	0.0667	-0.009
0.9144	0.0003		+E-02	0.2676	-E-01		-E-02	0.2000	-0.008
0.9156	0.0004		+E-02	0.3732	+E-01		-E-02	0.2667	-0.007
0.9175	0.0005		+E-02	0.9225	+E 00		-E-02	0.3333	-0.006
0.9188	0.0006		+E-02	1.0000	+E+01		-E-02	0.4000	-0.005
0.9200	0.0007		+E-01	0.0194	-E+01		-E-02	0.6667	-0.004
0.9203	0.0008		+E-01	0.0291	-E 00		-E-02	0.7333	-0.003
0.9225	0.0009		+E-01	0.0388	-E-02		-E-02	0.8000	-0.002
0.9231	0.0010		+E-01	0.2718	+E 00		-E-02	1.0000	-0.001
0.9319	0.0020		+E-01	1.0000	+E+01		+E-02	0.	0.001
0.9388	0.0030						+E-02	0.1538	0.002
0.9460	0.0040						+E-02	0.3846	0.003
0.9514	0.0050						+E-02	0.4615	0.004
0.9551	0.0060						+E-02	0.6154	0.005
0.9580	0.0070						+E-02	0.6923	0.006
0.9605	0.0080						+E-02	0.8462	0.007
0.9646	0.0090						+E-02	0.9231	0.009
0.9677	0.0100						+E-02	1.0000	0.010
0.9831	0.0200						+E-01	0.	0.010
0.9893	0.0300						+E-01	0.2143	0.020
0.9944	0.0400						+E-01	0.3571	0.030
0.9975	0.0500						+E-01	0.4643	0.040
0.9978	0.0600						+E-01	0.5536	0.050
0.9994	0.0700						+E-01	0.6429	0.060
0.9997	0.0800						+E-01	0.6964	0.070
1.0000	0.0900						+E-01	0.7500	0.080
							+E-01	0.8929	0.090
							+E-01	1.0000	0.100
							+E 00	0.	0.100
							+E 00	0.2240	0.200
							+E 00	0.3600	0.300
							+E 00	0.4960	0.400
							+E 00	0.6080	0.500
							+E 00	0.6720	0.600
							+E 00	0.7840	0.700
							+E 00	0.8400	0.800
							+E 00	0.9440	0.900
							+E 00	1.0000	1.000
							+E+01	0.	1.000
							+E+01	0.5568	2.000
							+E+01	0.7841	3.000
							+E+01	0.8977	4.000
							+E+01	0.9432	5.000
							+E+01	0.9773	6.000
							+E+01	0.9886	7.000
							+E+01	1.0000	8.000

SET 23 HBC = (0.9990)DE , MBC2 = 0. , T = 1800.

ZH	DELHBC	*	DELHBC RANGE	ZHM	DELMBC2 RANGE	*	DELMBC2 RANGE	ZM	DELMBC2
******	*******	*	*****	******	*****	*	*****	******	*******
0.	-0.0100		-E-02	0.1000	0		+E-02	0.	0.001
0.0007	-0.0090		-E-02	0.7000	+E-01		+E-02	0.2821	0.002
0.0013	-0.0020		-E-02	1.0000	+E 00		+E-02	0.4359	0.003
0.0066	-0.0010		-E-03	0.1600	0		+E-02	0.5824	0.004
0.0072	-0.0009		-E-03	0.5300	+E-02		+E-02	0.6593	0.005
0.0086	-0.0008		-E-03	0.8700	+E-01		+E-02	0.7692	0.006
0.0099	-0.0007		-E-03	1.0000	+E 00		+E-02	0.8315	0.007
0.0105	-0.0006		0	0.6860	0		+E-02	0.9084	0.008
0.0132	-0.0005		0	0.8681	+E-02		+E-02	0.9487	0.009
0.0178	-0.0004		0	0.9937	+E-01		+E-02	1.0000	0.010
0.0263	-0.0003		0	1.0000	+E 00		+E-01	0.	0.010
0.0408	-0.0002		+E-03	0.2000	0		+E-01	0.3185	0.020
0.0724	-0.0001		+E-03	0.4762	+E-02		+E-01	0.5074	0.030
0.0725	0.		+E-03	0.7833	+E-01		+E-01	0.6630	0.040
0.4918	0.		+E-03	1.0000	+E 00		+E-01	0.7926	0.050
0.4919	0.0001		+E-02	0.0190	+E-02		+E-01	0.8519	0.060
0.5760	0.0002		+E-02	0.1048	+E-01		+E-01	0.9148	0.070
0.6274	0.0003		+E-02	0.3762	+E 00		+E-01	0.9630	0.080
0.6675	0.0004		+E-02	1.0000	+E+01		+E-01	0.9778	0.090
0.6932	0.0005		+E-01	0.0211	+E-01		+E-01	1.0000	0.100
0.7149	0.0006		+E-01	0.1338	+E 00		+E 00	0.	0.100
0.7301	0.0007		+E-01	0.8239	+E+01		+E 00	0.2772	0.200
0.7446	0.0008		+E-01	1.0000	+E+02		+E 00	0.4239	0.300
0.7584	0.0009						+E 00	0.5489	0.400
0.7683	0.0010						+E 00	0.6739	0.500
0.8065	0.0020						+E 00	0.7609	0.600
0.8255	0.0030						+E 00	0.8478	0.700
0.8394	0.0040						+E 00	0.9348	0.800
0.8512	0.0050						+E 00	0.9728	0.900
0.8650	0.0060						+E 00	1.0000	1.000
0.8815	0.0070						+E+01	0.	1.000
0.8901	0.0080						+E+01	0.2620	2.000
0.8986	0.0090						+E+01	0.4978	3.000
0.9065	0.0100						+E+01	0.6507	4.000
0.9585	0.0200						+E+01	0.7729	5.000
0.9776	0.0300						+E+01	0.8428	6.000
0.9855	0.0400						+E+01	0.8952	7.000
0.9941	0.0500						+E+01	0.9258	8.000
0.9974	0.0600						+E+01	0.9607	9.000
0.9993	0.0700						+E+01	1.0000	10.000
1.0000	0.0900						+E+02	0.	10.000
							+E+02	1.0000	20.000

SET 24 HBC = (1.0090)DE , MBC2 = 1.00 , T = 1800.

ZH	DELHBC	*	DELHBC RANGE	ZHM	DELMBC2 RANGE	*	DELMBC2 RANGE	ZM	DELMBC2
******	*******	*	*****	******	*****	*	*****	******	*******
0.	-0.0050		-E-02	0.9077	-E 00		-E 00	0.	-1.000
0.0033	-0.0040		-E-02	0.9692	-E-01		-E 00	0.0261	-0.900
0.0053	-0.0030		-E-02	0.9846	+E-01		-E 00	0.0739	-0.800
0.0185	-0.0020		-E-02	1.0000	+E 00		-E 00	0.1174	-0.700
0.0428	-0.0010		-E-03	0.4381	-E 00		-E 00	0.1391	-0.600
0.0474	-0.0009		-E-03	0.7478	-E-01		-E 00	0.2087	-0.500
0.0533	-0.0008		-E-03	0.7832	-E-02		-E 00	0.2565	-0.400
0.0645	-0.0007		-E-03	0.7876	0		-E 00	0.3652	-0.300
0.0797	-0.0006		-E-03	0.8097	+E-02		-E 00	0.5957	-0.200
0.0928	-0.0005		-E-03	0.8938	+E-01		-E 00	1.0000	-0.100
0.1060	-0.0004		-E-03	1.0000	+E 00		-E-01	0.	-0.100
0.1244	-0.0003		0	0.0400	-E 00		-E-01	0.0664	-0.090
0.1468	-0.0002		0	0.2705	-E-01		-E-01	0.1055	-0.080
0.1916	-0.0001		0	0.4762	-E-02		-E-01	0.1445	-0.070
0.1917	0.		0	0.6286	0		-E-01	0.2461	-0.060
0.5372	0.		0	0.8400	+E-02		-E-01	0.3281	-0.050
0.5373	0.0001		0	0.9771	+E-01		-E-01	0.4180	-0.040
0.6090	0.0002		0	1.0000	+E 00		-E-01	0.5586	-0.030
0.6425	0.0003		+E-03	0.0909	-E 00		-E-01	0.7617	-0.020
0.6735	0.0004		+E-03	0.2493	-E-01		-E-01	1.0000	-0.010
0.6945	0.0005		+E-03	0.3050	-E-02		-E-02	0.	-0.010
0.7103	0.0006		+E-03	0.3109	0		-E-02	0.0809	-0.009
0.7248	0.0007		+E-03	0.3578	+E-02		-E-02	0.1324	-0.008
0.7360	0.0008		+E-03	0.6598	+E-01		-E-02	0.2132	-0.007
0.7465	0.0009		+E-03	0.9971	+E 00		-E-02	0.3162	-0.006
0.7617	0.0010		+E-03	1.0000	+E+01		-E-02	0.3897	-0.005
0.8117	0.0020		+E-02	0.0694	-E 00		-E-02	0.4632	-0.004
0.8302	0.0030		+E-02	0.0833	-E-01		-E-02	0.6103	-0.003
0.8446	0.0040		+E-02	0.0880	0		-E-02	0.8162	-0.002
0.8604	0.0050		+E-02	0.0972	+E-02		-E-02	1.0000	-0.001
0.8723	0.0060		+E-02	0.1343	+E-01		+E-02	0.	0.001
0.8822	0.0070		+E-02	0.4861	+E 00		+E-02	0.2015	0.002
0.8927	0.0080		+E-02	1.0000	+E+01		+E-02	0.3881	0.003
0.8986	0.0090		+E-01	0.0342	-E 00		+E-02	0.5597	0.004
0.9039	0.0100		+E-01	0.0616	-E-01		+E-02	0.6418	0.005
0.9526	0.0200		+E-01	0.0685	-E-02		+E-02	0.7463	0.006
0.9756	0.0300		+E-01	0.1027	+E 00		+E-02	0.8209	0.007
0.9842	0.0400		+E-01	0.8219	+E+01		+E-02	0.8881	0.008
0.9934	0.0500		+E-01	1.0000	+E+02		+E-02	0.9478	0.009
0.9974	0.0600						+E-02	1.0000	0.010
0.9987	0.0700						+E-01	0.	0.010
1.0000	0.0800						+E-01	0.2414	0.020
							+E-01	0.4236	0.030
							+E-01	0.5419	0.040
							+E-01	0.6995	0.050
							+E-01	0.7833	0.060
							+E-01	0.8424	0.070
							+E-01	0.8768	0.080
							+E-01	0.9507	0.090
							+E-01	1.0000	0.100
							+E 00	0.	0.100
							+E 00	0.2876	0.200
							+E 00	0.4506	0.300
							+E 00	0.6052	0.400
							+E 00	0.6953	0.500
							+E 00	0.7597	0.600
							+E 00	0.8069	0.700
							+E 00	0.8670	0.800
							+E 00	0.9056	0.900
							+E 00	1.0000	1.000
							+E+01	0.	1.000
							+E+01	0.2535	2.000
							+E+01	0.4470	3.000
							+E+01	0.5853	4.000
							+E+01	0.6959	5.000
							+E+01	0.7926	6.000
							+E+01	0.8664	7.000
							+E+01	0.9217	8.000
							+E+01	0.9631	9.000
							+E+01	1.0000	10.000
							+E+02	0.	10.000
							+E+02	1.0000	20.000

SET 25 : HBC = (1.0290)DE , MBC2 = 3.00 , T = 1800.

ZH	DELHBC	*	DELHBC RANGE	ZHM	DELMBC2 RANGE	*	DELMBC2 RANGE	ZM	DELMBC2
******	*******	*	*****	******	*****	*	*****	******	*******
0.	-0.0200		-E-01	1.0000	-E+01		-E+01	0.	-3.000
0.0007	-0.0100		-E-02	0.3925	-E+01		-E+01	0.3922	-2.000
0.0033	-0.0090		-E-02	0.8441	-E 00		-E+01	1.0000	-1.000
0.0066	-0.0080		-E-02	0.8763	-E-01		-E 00	0.	-1.000
0.0092	-0.0070		-E-02	0.9086	+E-01		-E 00	0.0430	-0.900
0.0145	-0.0060		-E-02	0.9946	+E 00		-E 00	0.0938	-0.800
0.0230	-0.0050		-E-02	1.0000	+E+01		-E 00	0.1367	-0.700
0.0316	-0.0040		-E-03	0.0458	-E+01		-E 00	0.2188	-0.600
0.0434	-0.0030		-E-03	0.5125	-E 00		-E 00	0.2930	-0.500
0.0724	-0.0020		-E-03	0.8208	-E-01		-E 00	0.3906	-0.400
0.1231	-0.0010		-E-03	0.8292	-E-02		-E 00	0.5430	-0.300
0.1317	-0.0009		-E-03	0.8333	+E-02		-E 00	0.7344	-0.200
0.1415	-0.0008		-E-03	0.8917	+E-01		-E 00	1.0000	-0.100
0.1494	-0.0007		-E-03	0.9958	+E 00		-E-01	0.	-0.100
0.1600	-0.0006		-E-03	1.0000	+E+01		-E-01	0.0504	-0.090
0.1731	-0.0005		0	0.0064	-E+01		-E-01	0.1176	-0.080
0.1955	-0.0004		0	0.0362	-E 00		-E-01	0.1933	-0.070
0.2146	-0.0003		0	0.3028	-E-01		-E-01	0.2395	-0.060
0.2416	-0.0002		0	0.5096	-E-02		-E-01	0.3487	-0.050
0.2811	-0.0001		0	0.6418	0		-E-01	0.4496	-0.040
0.2812	0.		0	0.8060	+E-02		-E-01	0.5966	-0.030
0.5899	0.		0	0.9808	+E-01		-E-01	0.7395	-0.020
0.5900	0.0001		0	1.0000	+E 00		-E-01	1.0000	-0.010
0.6406	0.0002		+E-03	0.0142	-E+01		-E-02	0.	-0.010
0.6774	0.0003		+E-03	0.1139	-E 00		-E-02	0.0741	-0.009
0.7031	0.0004		+E-03	0.2242	-E-01		-E-02	0.1667	-0.008
0.7182	0.0005		+E-03	0.2562	-E-02		-E-02	0.2500	-0.007
0.7307	0.0006		+E-03	0.2598	0		-E-02	0.3333	-0.006
0.7485	0.0007		+E-03	0.2918	+E-02		-E-02	0.4352	-0.005
0.7525	0.0008		+E-03	0.6228	+E-01		-E-02	0.6111	-0.004
0.7617	0.0009		+E-03	0.9715	+E 00		-E-02	0.7500	-0.003
0.7749	0.0010		+E-03	1.0000	+E+01		-E-02	0.8889	-0.002
0.8229	0.0020		+E-02	0.0524	-E+01		-E-02	1.0000	-0.001
0.8486	0.0030		+E-02	0.1152	-E 00		+E-02	0.	0.001
0.8578	0.0040		+E-02	0.1204	-E-01		+E-02	0.1609	0.002
0.8697	0.0050		+E-02	0.1414	+E-01		+E-02	0.3678	0.003
0.8776	0.0060		+E-02	0.5602	+E 00		+E-02	0.5862	0.004
0.8841	0.0070		+E-02	1.0000	+E+01		+E-02	0.6667	0.005
0.8947	0.0080		+E-01	0.0397	-E 00		+E-02	0.7586	0.006
0.8953	0.0090		+E-01	0.0464	-E-01		+E-02	0.8161	0.007
0.9006	0.0100		+E-01	0.0530	+E-01		+E-02	0.8506	0.008
0.9473	0.0200		+E-01	0.0795	+E 00		+E-02	0.9195	0.009
0.9730	0.0300		+E-01	0.7815	+E+01		+E-02	1.0000	0.010
0.9868	0.0400		+E-01	1.0000	+E+02		+E-01	0.	0.010
0.9928	0.0500						+E-01	0.2350	0.020
0.9961	0.0600						+E-01	0.3900	0.030
0.9980	0.0700						+E-01	0.5450	0.040
1.0000	0.0800						+E-01	0.6350	0.050
							+E-01	0.7700	0.060
							+E-01	0.8000	0.070
							+E-01	0.8700	0.080
							+E-01	0.9550	0.090
							+E-01	1.0000	0.100
							+E 00	0.	0.100
							+E 00	0.2672	0.200
							+E 00	0.4353	0.300
							+E 00	0.5991	0.400
							+E 00	0.6897	0.500
							+E 00	0.7888	0.600
							+E 00	0.8621	0.700
							+E 00	0.9009	0.800
							+E 00	0.9526	0.900
							+E 00	1.0000	1.000
							+E+01	0.	1.000
							+E+01	0.2300	2.000
							+E+01	0.3700	3.000
							+E+01	0.5300	4.000
							+E+01	0.6450	5.000
							+E+01	0.7600	6.000
							+E+01	0.8400	7.000
							+E+01	0.9100	8.000
							+E+01	0.9400	9.000
							+E+01	1.0000	10.000
							+E+02	0.	10.000
							+E+02	1.0000	20.000

SET 26 HBC = (1.0590)DE , MBC2 = 6.00 ; T = 1800.

ZH	DELHBC	*	DELHBC RANGE	ZHM	DELMBC2 RANGE	*	DELMBC2 RANGE	ZM	DELMBC2
******	*******	*	*****	******	*****	*	*****	******	*******
0.	-0.0300		-E-01	1.0000	-E+01		-E+01	0.	-6.000
0.0007	-0.0200		-E-02	0.3694	-E+01		-E+01	0.1569	-5.000
0.0257	-0.0100		-E-02	0.8153	-E 00		-E+01	0.3137	-4.000
0.0303	-0.0090		-E-02	0.8288	-E-01		-E+01	0.4771	-3.000
0.0369	-0.0080		-E-02	0.8333	-E-02		-E+01	0.6601	-2.000
0.0441	-0.0070		-E-02	0.8378	+E-02		-E+01	1.0000	-1.000
0.0527	-0.0060		-E-02	0.8649	+E-01		-E 00	0.	-1.000
0.0606	-0.0050		-E-02	0.9595	+E 00		-E 00	0.0453	-0.900
0.0665	-0.0040		-E-02	1.0000	+E+01		-E 00	0.0981	-0.800
0.0836	-0.0030		-E-03	0.0337	-E+01		-E 00	0.1925	-0.700
0.1119	-0.0020		-E-03	0.4644	-E 00		-E 00	0.2679	-0.600
0.1718	-0.0010		-E-03	0.7753	-E-01		-E 00	0.3434	-0.500
0.1797	-0.0009		-E-03	0.7978	-E-02		-E 00	0.4377	-0.400
0.1876	-0.0008		-E-03	0.8052	+E-02		-E 00	0.5736	-0.300
0.1962	-0.0007		-E-03	0.8577	+E-01		-E 00	0.7094	-0.200
0.2087	-0.0006		-E-03	0.9813	+E 00		-E 00	1.0000	-0.100
0.2238	-0.0005		-E-03	1.0000	+E+01		-E-01	0.	-0.100
0.2416	-0.0004		0	0.0390	-E 00		-E-01	0.0487	-0.090
0.2640	-0.0003		0	0.3098	-E-01		-E-01	0.1018	-0.080
0.2897	-0.0002		0	0.5049	-E-02		-E-01	0.1770	-0.070
0.3476	-0.0001		0	0.6244	0		-E-01	0.2566	-0.060
0.3477	0.		0	0.8024	+E-02		-E-01	0.3407	-0.050
0.6175	0.		0	0.9707	+E-01		-E-01	0.4558	-0.040
0.6176	0.0001		0	1.0000	+E 00		-E-01	0.5575	-0.030
0.6570	0.0002		+E-03	0.0210	-E+01		-E-01	0.7389	-0.020
0.6919	0.0003		+E-03	0.0840	-E 00		-E-01	1.0000	-0.010
0.7077	0.0004		+E-03	0.1933	-E-01		-E-02	0.	-0.010
0.7202	0.0005		+E-03	0.2017	-E-02		-E-02	0.0674	-0.009
0.7360	0.0006		+E-03	0.2395	+E-02		-E-02	0.1348	-0.008
0.7465	0.0007		+E-03	0.5504	+E-01		-E-02	0.2472	-0.007
0.7551	0.0008		+E-03	0.9622	+E 00		-E-02	0.3146	-0.006
0.7663	0.0009		+E-03	1.0000	+E+01		-E-02	0.4719	-0.005
0.7742	0.0010		+E-02	0.0471	-E+01		-E-02	0.5618	-0.004
0.8223	0.0020		+E-02	0.1152	-E 00		-E-02	0.6742	-0.003
0.8525	0.0030		+E-02	0.1204	-E-01		-E-02	0.8202	-0.002
0.8650	0.0040		+E-02	0.1257	0		-E-02	1.0000	-0.001
0.8716	0.0050		+E-02	0.1518	+E-01		+E-02	0.	0.001
0.8776	0.0060		+E-02	0.5602	+E 00		+E-02	0.1765	0.002
0.8841	0.0070		+E-02	1.0000	+E+01		+E-02	0.3647	0.003
0.8901	0.0080		+E-01	0.0596	-E+01		+E-02	0.4706	0.004
0.8960	0.0090		+E-01	0.1060	-E 00		+E-02	0.5765	0.005
0.8999	0.0100		+E-01	0.1192	-E-01		+E-02	0.7647	0.006
0.9473	0.0200		+E-01	0.1258	+E-01		+E-02	0.8471	0.007
0.9737	0.0300		+E-01	0.1391	+E 00		+E-02	0.9176	0.008
0.9868	0.0400		+E-01	0.7947	+E+01		+E-02	0.9647	0.009
0.9934	0.0500		+E-01	1.0000	+E+02		+E-02	1.0000	0.010
0.9961	0.0600		+E 00	1.0000	+E+02		+E-01	0.	0.010
0.9980	0.0700						+E-01	0.2604	0.020
0.9987	0.0900						+E-01	0.4083	0.030
0.9993	0.1000						+E-01	0.5266	0.040
1.0000	0.2000						+E-01	0.6450	0.050
							+E-01	0.7515	0.060
							+E-01	0.7929	0.070
							+E-01	0.8757	0.080
							+E-01	0.9349	0.090
							+E-01	1.0000	0.100
							+E 00	0.	0.100
							+E 00	0.2500	0.200
							+E 00	0.4303	0.300
							+E 00	0.5820	0.400
							+E 00	0.6926	0.500
							+E 00	0.7705	0.600
							+E 00	0.8361	0.700
							+E 00	0.9098	0.800
							+E 00	0.9631	0.900
							+E 00	1.0000	1.000
							+E+01	0.	1.000
							+E+01	0.2816	2.000
							+E+01	0.4175	3.000
							+E+01	0.5097	4.000
							+E+01	0.6456	5.000
							+E+01	0.7136	6.000
							+E+01	0.8252	7.000
							+E+01	0.8835	8.000
							+E+01	0.9466	9.000
							+E+01	1.0000	10.000
							+E+02	0.	10.000
							+E+02	1.0000	20.000

SET 27 HBC = (1.0990)DE , MBC2 = 10.00 , T = 1800.

ZH	DELHBC	*	DELHBC RANGE	ZHM	DELMBC2	*	DELMBC2 RANGE	ZM	DELMBC2
******	*******	*	*****	******	*****	*	*****	******	*******
0.	-0.0400		-E-01	0.9899	-E+01		-E+01	0.	-10.000
0.0033	-0.0300		-E-01	1.0000	-E 00		-E+01	0.0563	-9.000
0.0233	-0.0200		-E-02	0.3717	-E+01		-E+01	0.1127	-8.000
0.0652	-0.0100		-E-02	0.8325	-E 00		-E+01	0.1972	-7.000
0.0731	-0.0090		-E-02	0.8534	-E-01		-E+01	0.2723	-6.000
0.0757	-0.0080		-E-02	0.8743	+E-01		-E+01	0.3944	-5.000
0.0843	-0.0070		-E-02	0.9424	+E 00		-E+01	0.5023	-4.000
0.0876	-0.0060		-E-02	1.0000	+E+01		-E+01	0.6103	-3.000
0.0948	-0.0050		-E-03	0.0369	-E+01		-E+01	0.7418	-2.000
0.1066	-0.0040		-E-03	0.4391	-E 00		-E+01	1.0000	-1.000
0.1231	-0.0030		-E-03	0.8118	-E-01		-E 00	0.	-1.000
0.1475	-0.0020		-E-03	0.8303	-E-02		-E 00	0.0361	-0.900
0.1909	-0.0010		-E-03	0.8450	+E-02		-E 00	0.0803	-0.800
0.1949	-0.0009		-E-03	0.9041	+E-01		-E 00	0.1245	-0.700
0.2054	-0.0008		-E-03	0.9963	+E 00		-E 00	0.1968	-0.600
0.2140	-0.0007		-E-03	1.0000	+E+01		-E 00	0.2530	-0.500
0.2251	-0.0006		0	0.0180	-E 00		-E 00	0.3574	-0.400
0.2363	-0.0005		0	0.2552	-E-01		-E 00	0.4900	-0.300
0.2535	-0.0004		0	0.4716	-E-02		-E 00	0.6867	-0.200
0.2739	-0.0003		0	0.6057	0		-E 00	1.0000	-0.100
0.3120	-0.0002		0	0.7809	+E-02		-E-01	0.	-0.100
0.3693	-0.0001		0	0.9510	+E-01		-E-01	0.0605	-0.090
0.3694	0.		0	0.9974	+E 00		-E-01	0.1163	-0.080
0.6248	0.		0	1.0000	+E+01		-E-01	0.1767	-0.070
0.6249	0.0001		+E-03	0.0278	-E+01		-E-01	0.2512	-0.060
0.6629	0.0002		+E-03	0.1250	-E 00		-E-01	0.3395	-0.050
0.6853	0.0003		+E-03	0.1806	-E-01		-E-01	0.4326	-0.040
0.6991	0.0004		+E-03	0.1944	-E-02		-E-01	0.5488	-0.030
0.7103	0.0005		+E-03	0.2037	0		-E-01	0.7581	-0.020
0.7268	0.0006		+E-03	0.2407	+E-02		-E-01	1.0000	-0.010
0.7373	0.0007		+E-03	0.6019	+E-01		-E-02	0.	-0.010
0.7485	0.0008		+E-03	0.9815	+E 00		-E-02	0.0870	-0.009
0.7584	0.0009		+E-03	1.0000	+E+01		-E-02	0.1957	-0.008
0.7670	0.0010		+E-02	0.0856	-E+01		-E-02	0.2826	-0.007
0.8302	0.0020		+E-02	0.1757	-E 00		-E-02	0.3587	-0.006
0.8552	0.0030		+E-02	0.2027	-E-01		-E-02	0.4239	-0.005
0.8723	0.0040		+E-02	0.2072	0		-E-02	0.5326	-0.004
0.8835	0.0050		+E-02	0.2297	+E-01		-E-02	0.7283	-0.003
0.8907	0.0060		+E-02	0.5676	+E 00		-E-02	0.8696	-0.002
0.8973	0.0070		+E-02	1.0000	+E+01		-E-02	1.0000	-0.001
0.9026	0.0080		+E-01	0.0692	-E+01		+E-02	0.	0.001
0.9065	0.0090		+E-01	0.0923	-E 00		+E-02	0.1375	0.002
0.9131	0.0100		+E-01	0.1000	+E-01		+E-02	0.2875	0.003
0.9506	0.0200		+E-01	0.1308	+E 00		+E-02	0.4125	0.004
0.9743	0.0300		+E-01	0.7692	+E+01		+E-02	0.5375	0.005
0.9835	0.0400		+E-01	1.0000	+E+02		+E-02	0.6125	0.006
0.9901	0.0500		+E 00	1.0000	+E+02		+E-02	0.7250	0.007
0.9947	0.0600						+E-02	0.8250	0.008
0.9967	0.0700						+E-02	0.9125	0.009
0.9974	0.0800						+E-02	1.0000	0.010
0.9987	0.0900						+E-01	0.	0.010
1.0000	0.2000						+E-01	0.2353	0.020
							+E-01	0.4059	0.030
							+E-01	0.5647	0.040
							+E-01	0.6647	0.050
							+E-01	0.7471	0.060
							+E-01	0.7941	0.070
							+E-01	0.8824	0.080
							+E-01	0.9353	0.090
							+E-01	1.0000	0.100
							+E 00	0.	0.100
							+E 00	0.2995	0.200
							+E 00	0.4055	0.300
							+E 00	0.5300	0.400
							+E 00	0.6636	0.500
							+E 00	0.7419	0.600
							+E 00	0.8387	0.700
							+E 00	0.8986	0.800
							+E 00	0.9493	0.900
							+E 00	1.0000	1.000
							+E+01	0.	1.000
							+E+01	0.2908	2.000
							+E+01	0.4643	3.000
							+E+01	0.6020	4.000
							+E+01	0.6990	5.000
							+E+01	0.7653	6.000
							+E+01	0.8163	7.000
							+E+01	0.8929	8.000
							+E+01	0.9745	9.000
							+E+01	1.0000	10.000
							+E+02	0.	10.000
							+E+02	1.0000	20.000

SET 28 HBC = (1.1240)DE , MBC2 = 12.50 , T = 1800.

ZH	DELHBC	*	DELHBC RANGE	ZHM	DELMBC2	*	DELMBC2 RANGE	ZM	DELMBC2
******	*******	*	*****	******	*****	*	*****	******	*******
0.	-0.0500		-E-01	0.1037	-E+02		-E+02	0.	-12.500
0.0066	-0.0400		-E-01	1.0000	-E+01		-E+02	1.0000	-10.000
0.0184	-0.0300		-E-02	0.3846	-E+01		-E+01	0.	-10.000
0.0434	-0.0200		-E-02	0.8769	-E 00		-E+01	0.0586	-9.000
0.0889	-0.0100		-E-02	0.9077	-E-01		-E+01	0.1216	-8.000
0.0915	-0.0090		-E-02	0.9282	+E-01		-E+01	0.1712	-7.000
0.1020	-0.0080		-E-02	0.9846	+E 00		-E+01	0.2613	-6.000
0.1080	-0.0070		-E-02	1.0000	+E+01		-E+01	0.3288	-5.000
0.1172	-0.0060		-E-03	0.0233	-E+01		-E+01	0.4640	-4.000
0.1297	-0.0050		-E-03	0.4698	-E 00		-E+01	0.6126	-3.000
0.1356	-0.0040		-E-03	0.8930	-E-01		-E+01	0.7838	-2.000
0.1540	-0.0030		-E-03	0.8977	0		-E+01	1.0000	-1.000
0.1764	-0.0020		-E-03	0.9163	+E-02		-E 00	0.	-1.000
0.2172	-0.0010		-E-03	0.9442	+E-01		-E 00	0.0474	-0.900
0.2258	-0.0009		-E-03	0.9953	+E 00		-E 00	0.0862	-0.800
0.2304	-0.0008		-E-03	1.0000	+E+01		-E 00	0.1466	-0.700
0.2370	-0.0007		0	0.0047	-E+01		-E 00	0.1940	-0.600
0.2442	-0.0006		0	0.0306	-E 00		-E 00	0.2543	-0.500
0.2541	-0.0005		0	0.2918	-E-01		-E 00	0.3491	-0.400
0.2673	-0.0004		0	0.5200	-E-02		-E 00	0.4828	-0.300
0.2923	-0.0003		0	0.6306	0		-E 00	0.6595	-0.200
0.3107	-0.0002		0	0.8518	+E-02		-E 00	1.0000	-0.100
0.3588	-0.0001		0	0.9859	+E-01		-E-01	0.	-0.100
0.3589	0.		0	0.9976	+E 00		-E-01	0.0087	-0.090
0.6386	0.		0	1.0000	+E+01		-E-01	0.0568	-0.080
0.6387	0.0001		+E-03	0.0158	-E+01		-E-01	0.1179	-0.070
0.6893	0.0002		+E-03	0.0949	-E 00		-E-01	0.1965	-0.060
0.7209	0.0003		+E-03	0.1700	-E-01		-E-01	0.2838	-0.050
0.7433	0.0004		+E-03	0.1937	-E-02		-E-01	0.3886	-0.040
0.7604	0.0005		+E-03	0.2016	0		-E-01	0.5066	-0.030
0.7735	0.0006		+E-03	0.2253	+E-02		-E-01	0.6943	-0.020
0.7847	0.0007		+E-03	0.6957	+E-01		-E-01	1.0000	-0.010
0.7946	0.0008		+E-03	0.9763	+E 00		-E-02	0.	-0.010
0.7992	0.0009		+E-03	1.0000	+E+01		-E-02	0.0583	-0.009
0.8051	0.0010		+E-02	0.0628	-E+01		-E-02	0.1165	-0.008
0.8492	0.0020		+E-02	0.0942	-E 00		-E-02	0.2621	-0.007
0.8749	0.0030		+E-02	0.1047	-E-01		-E-02	0.3495	-0.006
0.8907	0.0040		+E-02	0.1152	+E-01		-E-02	0.4951	-0.005
0.9052	0.0050		+E-02	0.6126	+E 00		-E-02	0.6117	-0.004
0.9111	0.0060		+E-02	1.0000	+E+01		-E-02	0.7087	-0.003
0.9151	0.0070		+E-01	0.0291	-E+01		-E-02	0.8447	-0.002
0.9197	0.0080		+E-01	0.0583	-E 00		-E-02	1.0000	-0.001
0.9250	0.0090		+E-01	0.0680	+E-01		+E-02	0.	0.001
0.9309	0.0100		+E-01	0.1068	+E 00		+E-02	0.2115	0.002
0.9572	0.0200		+E-01	0.8932	+E+01		+E-02	0.3173	0.003
0.9776	0.0300		+E-01	1.0000	+E+02		+E-02	0.4038	0.004
0.9901	0.0400		+E 00	1.0000	+E+02		+E-02	0.5288	0.005
0.9928	0.0500						+E-02	0.6250	0.006
0.9934	0.0600						+E-02	0.7019	0.007
0.9954	0.0700						+E-02	0.8173	0.008
0.9967	0.0800						+E-02	0.9327	0.009
0.9980	0.0900						+E-02	1.0000	0.010
0.9987	0.1000						+E-01	0.	0.010
1.0000	0.2000						+E-01	0.2540	0.020
							+E-01	0.4656	0.030
							+E-01	0.5820	0.040
							+E-01	0.7090	0.050
							+E-01	0.7725	0.060
							+E-01	0.8360	0.070
							+E-01	0.9259	0.080
							+E-01	0.9683	0.090
							+E-01	1.0000	0.100
							+E 00	0.	0.100
							+E 00	0.2843	0.200
							+E 00	0.4467	0.300
							+E 00	0.5888	0.400
							+E 00	0.6751	0.500
							+E 00	0.7563	0.600
							+E 00	0.8426	0.700
							+E 00	0.8934	0.800
							+E 00	0.9645	0.900
							+E 00	1.0000	1.000
							+E+01	0.	1.000
							+E+01	0.3554	2.000
							+E+01	0.5783	3.000
							+E+01	0.6627	4.000
							+E+01	0.7410	5.000
							+E+01	0.8012	6.000
							+E+01	0.8735	7.000
							+E+01	0.9277	8.000
							+E+01	0.9639	9.000
							+E+01	1.0000	10.000
							+E+02	0.	10.000
							+E+02	1.0000	20.000

SET 29 HBC = (1.1490)DE , MBC2 = 15.CO , T = 1800.

ZH	DELHBC	*	DELHBC RANGE	ZHM	DELMBC2	*	DELMBC2 RANGE	ZM	DELMBC2
******	*******	*	*****	******	*****	*	*****	******	*******
0.	-0.3000		-E 00	0.5556	-E+02		-E+02	0.	-15.000
0.0026	-0.2000		-E 00	1.0000	-E+01		-E+02	1.0000	-10.000
0.0118	-0.1000		-E-01	0.1262	-E+02		-E+01	0.	-10.000
0.0138	-0.0900		-E-01	0.8883	-E+01		-E+01	0.0476	-9.000
0.0171	-0.0800		-E-01	0.9417	-E 00		-E+01	0.1476	-8.000
0.0257	-0.0700		-E-01	0.9612	+E 00		-E+01	0.2048	-7.000
0.0329	-0.0600		-E-01	1.0000	+E+01		-E+01	0.2714	-6.000
0.0487	-0.0500		-E-02	0.2816	-E+01		-E+01	0.4000	-5.000
0.0671	-0.0400		-E-02	0.7282	-E 00		-E+01	0.4905	-4.000
0.0882	-0.0300		-E-02	0.8252	-E-01		-E+01	0.6190	-3.000
0.1172	-0.0200		-E-02	0.8447	+E-01		-E+01	0.8000	-2.000
0.1475	-0.0100		-E-02	0.9320	+E 00		-E+01	1.0000	-1.000
0.1488	-0.0090		-E-02	1.0000	+E+01		-E 00	0.	-1.000
0.1560	-0.0080		-E-03	0.0165	-E+01		-E 00	0.0506	-0.900
0.1606	-0.0070		-E-03	0.2088	-E 00		-E 00	0.0696	-0.800
0.1659	-0.0060		-E-03	0.4835	-E-01		-E 00	0.1266	-0.700
0.1738	-0.0050		-E-03	0.5055	-E-02		-E 00	0.1519	-0.600
0.1810	-0.0040		-E-03	0.5220	+E-02		-E 00	0.1899	-0.500
0.1863	-0.0030		-E-03	0.7363	+E-01		-E 00	0.2658	-0.400
0.1942	-0.0020		-E-03	1.0000	+E 00		-E 00	0.3734	-0.300
0.2153	-0.0010		0	0.0014	-E+01		-E 00	0.6646	-0.200
0.2186	-0.0009		0	0.0544	-E 00		-E 00	1.0000	-0.100
0.2225	-0.0008		0	0.3116	-E-01		-E-01	0.	-0.100
0.2284	-0.0007		0	0.5020	-E-02		-E-01	0.0458	-0.090
0.2344	-0.0006		0	0.6082	0		-E-01	0.0810	-0.080
0.2429	-0.0005		0	0.7673	+E-02		-E-01	0.1514	-0.070
0.2541	-0.0004		0	0.9741	+E-01		-E-01	0.2183	-0.060
0.2653	-0.0003		0	1.0000	+E 00		-E-01	0.3028	-0.050
0.2864	-0.0002		+E-03	0.1739	-E 00		-E-01	0.3838	-0.040
0.3351	-0.0001		+E-03	0.4696	-E-01		-E-01	0.5352	-0.030
0.3352	0.		+E-03	0.5478	-E-02		-E-01	0.7007	-0.020
0.8190	0.		+E-03	0.5565	+E-02		-E-01	1.0000	-0.010
0.8191	0.0001		+E-03	0.7913	+E-01		-E-02	0.	-0.010
0.8473	0.0002		+E-03	1.0000	+E 00		-E-02	0.0523	-0.009
0.8558	0.0003		+E-02	0.0842	-E+01		-E-02	0.1111	-0.008
0.8697	0.0004		+E-02	0.1579	-E 00		-E-02	0.2222	-0.007
0.8789	0.0005		+E-02	0.1684	-E-01		-E-02	0.3268	-0.006
0.8835	0.0006		+E-02	0.1895	+E-02		-E-02	0.3987	-0.005
0.8868	0.0007		+E-02	0.3579	+E-01		-E-02	0.5033	-0.004
0.8894	0.0008		+E-02	0.8105	+E 00		-E-02	0.6797	-0.003
0.8920	0.0009		+E-02	1.0000	+E+01		-E-02	0.8562	-0.002
0.8947	0.0010		+E-01	0.0615	-E+01		-E-02	1.0000	-0.001
0.9151	0.0020		+E-01	0.0769	+E-01		+E-02	0.	0.001
0.9210	0.0030		+E-01	0.2154	+E 00		+E-02	0.1707	0.002
0.9289	0.0040		+E-01	0.9077	+E+01		+E-02	0.3333	0.003
0.9342	0.0050		+E-01	1.0000	+E+02		+E-02	0.4472	0.004
0.9401	0.0060						+E-02	0.5610	0.005
0.9440	0.0070						+E-02	0.6341	0.006
0.9473	0.0080						+E-02	0.7805	0.007
0.9533	0.0090						+E-02	0.8537	0.008
0.9572	0.0100						+E-02	0.9106	0.009
0.9770	0.0200						+E-02	1.0000	0.010
0.9882	0.0300						+E-01	0.	0.010
0.9914	0.0400						+E-01	0.2700	0.020
0.9947	0.0500						+E-01	0.4641	0.030
0.9954	0.0600						+E-01	0.6118	0.040
0.9974	0.0700						+E-01	0.6709	0.050
0.9980	0.0800						+E-01	0.7553	0.060
1.0000	0.1000						+E-01	0.8312	0.070
							+E-01	0.8945	0.080
							+E-01	0.9536	0.090
							+E-01	1.0000	0.100
							+E 00	0.	0.100
							+E 00	0.3782	0.200
							+E 00	0.6474	0.300
							+E 00	0.7244	0.400
							+E 00	0.8205	0.500
							+E 00	0.8718	0.600
							+E 00	0.9167	0.700
							+E 00	0.9359	0.800
							+E 00	0.9744	0.900
							+E 00	1.0000	1.000
							+E+01	0.	1.000
							+E+01	0.4103	2.000
							+E+01	0.6538	3.000
							+E+01	0.7821	4.000
							+E+01	0.8590	5.000
							+E+01	0.8974	6.000
							+E+01	0.9487	7.000
							+E+01	0.9872	8.000
							+E+01	1.0000	9.000
							+E+02	0.	10.000
							+E+02	1.0000	20.000

SET 30 HBC = (1.1990)DE , MBC2 = 20.00 , T = 1800.

ZH	DELHBC	*	DELHBC RANGE	ZHM	DELMBC2	*	DELMBC2 RANGE	ZM	DELMBC2
******	*******	*	*****	******	*****	*	*****	******	*******
0.	-0.3000		-E 00	0.5938	-E+02		-E+02	0.	-20.000
0.0020	-0.2000		-E 00	1.0000	-E+01		-E+02	1.0000	-10.000
0.0211	-0.1000		-E-01	0.1061	-E+02		-E+01	0.	-10.000
0.0237	-0.0900		-E-01	0.8535	-E+01		-E+01	0.0558	-9.000
0.0296	-0.0800		-E-01	0.9192	-E 00		-E+01	0.1117	-8.000
0.0382	-0.0700		-E-01	0.9293	-E-01		-E+01	0.1980	-7.000
0.0494	-0.0600		-E-01	0.9495	+E-01		-E+01	0.2690	-6.000
0.0612	-0.0500		-E-01	0.9798	+E 00		-E+01	0.3655	-5.000
0.0744	-0.0400		-E-01	1.0000	+E+01		-E+01	0.4975	-4.000
0.1001	-0.0300		-E-02	0.2105	-E+01		-E+01	0.6142	-3.000
0.1264	-0.0200		-E-02	0.5921	-E 00		-E+01	0.7817	-2.000
0.1514	-0.0100		-E-02	0.6711	-E-01		-E+01	1.0000	-1.000
0.1580	-0.0090		-E-02	0.7105	+E-01		-E 00	0.	-1.000
0.1600	-0.0080		-E-02	0.8947	+E 00		-E 00	0.0442	-0.900
0.1652	-0.0070		-E-02	1.0000	+E+01		-E 00	0.0885	-0.800
0.1679	-0.0060		-E-03	0.0071	-E+01		-E 00	0.1327	-0.700
0.1731	-0.0050		-E-03	0.1071	-E 00		-E 00	0.1947	-0.600
0.1777	-0.0040		-E-03	0.2429	-E-01		-E 00	0.2124	-0.500
0.1810	-0.0030		-E-03	0.3071	-E-02		-E 00	0.2566	-0.400
0.1876	-0.0020		-E-03	0.3214	+E-02		-E 00	0.3363	-0.300
0.2014	-0.0010		-E-03	0.6643	+E-01		-E 00	0.5310	-0.200
0.2028	-0.0009		-E-03	1.0000	+E 00		-E 00	1.0000	-0.100
0.2041	-0.0008		0	0.0076	-E 00		-E-01	0.	-0.100
0.2067	-0.0007		0	0.2217	-E-01		-E-01	0.0469	-0.090
0.2120	-0.0006		0	0.5146	-E-02		-E-01	0.1055	-0.080
0.2140	-0.0005		0	0.6140	0		-E-01	0.1680	-0.070
0.2251	-0.0004		0	0.8408	+E-02		-E-01	0.2031	-0.060
0.2403	-0.0003		0	0.9975	+E-01		-E-01	0.2656	-0.050
0.2581	-0.0002		0	0.9987	+E 00		-E-01	0.3672	-0.040
0.2936	-0.0001		0	1.0000	+E+01		-E-01	0.4688	-0.030
0.2937	0.		+E-03	0.0130	-E+01		-E-01	0.6172	-0.020
0.8104	0.		+E-03	0.2662	-E 00		-E-01	1.0000	-0.010
0.8105	0.0001		+E-03	0.6558	-E-01		-E-02	0.	-0.010
0.8492	0.0002		+E-03	0.6623	-E-02		-E-02	0.0542	-0.009
0.8664	0.0003		+E-03	0.7208	+E-02		-E-02	0.1375	-0.008
0.8756	0.0004		+E-03	0.8896	+E-01		-E-02	0.2167	-0.007
0.8887	0.0005		+E-03	0.9870	+E 00		-E-02	0.2708	-0.006
0.8980	0.0006		+E-03	1.0000	+E+01		-E-02	0.3667	-0.005
0.9019	0.0007		+E-02	0.1268	-E+01		-E-02	0.4958	-0.004
0.9052	0.0008		+E-02	0.2113	-E 00		-E-02	0.6542	-0.003
0.9085	0.0009		+E-02	0.2254	-E-01		-E-02	0.8083	-0.002
0.9118	0.0010		+E-02	0.2394	+E-02		-E-02	1.0000	-0.001
0.9276	0.0020		+E-02	0.3239	+E-01		+E-02	0.	0.001
0.9361	0.0030		+E-02	0.8732	+E 00		+E-02	0.1789	0.002
0.9421	0.0040		+E-02	1.0000	+E+01		+E-02	0.3421	0.003
0.9480	0.0050		+E-01	0.1270	-E+01		+E-02	0.4789	0.004
0.9519	0.0060		+E-01	0.2222	-E 00		+E-02	0.5842	0.005
0.9546	0.0070		+E-01	0.3333	+E 00		+E-02	0.6947	0.006
0.9566	0.0080		+E-01	1.0000	+E+01		+E-02	0.7737	0.007
0.9579	0.0090						+E-02	0.8474	0.008
0.9585	0.0100						+E-02	0.9211	0.009
0.9737	0.0200						+E-02	1.0000	0.010
0.9895	0.0300						+E-01	0.	0.010
0.9941	0.0400						+E-01	0.3619	0.020
0.9960	0.0500						+E-01	0.5714	0.030
0.9974	0.0600						+E-01	0.6619	0.040
0.9993	0.0800						+E-01	0.7238	0.050
1.0000	0.0900						+E-01	0.8143	0.060
							+E-01	0.8857	0.070
							+E-01	0.9429	0.080
							+E-01	0.9714	0.090
							+E-01	1.0000	0.100
							+E 00	0.	0.100
							+E 00	0.4651	0.200
							+E 00	0.6667	0.300
							+E 00	0.7674	0.400
							+E 00	0.8295	0.500
							+E 00	0.8682	0.600
							+E 00	0.9147	0.700
							+E 00	0.9535	0.800
							+E 00	0.9767	0.900
							+E 00	1.0000	1.000
							+E+01	0.	1.000
							+E+01	0.3788	2.000
							+E+01	0.5455	3.000
							+E+01	0.7273	4.000
							+E+01	0.8030	5.000
							+E+01	0.9394	6.000
							+E+01	0.9848	7.000
							+E+01	1.0000	8.000

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